U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

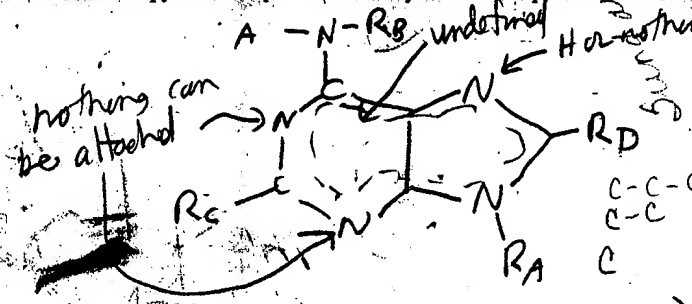
Requestor's Name: Berl

Serial Number: 10/740,653

Date: 6/15 6/17 Phone: 4778 Art Unit: 1624 405

Search Topic:

Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).

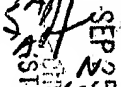


R_B, R_A = H/C

A, A' = H/CH_3

R_C, R_D = H/Hal/O/S/N/C

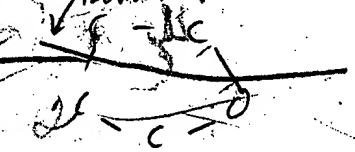
J = $(CH_2)_{1-6}$ or –C(=O)– or 

Q = CN/ N(A,A')/ $(CH_2)_{1-6}$ / S(=O)(=O)–N(A,A') / $(CH_2)_{0-6}$–N–C(=N)–N / 

With these provisos

1) There must be at least one P present

2) R_D cannot be –J–Q

3) R_A cannot be 

3) R_A cannot have exactly 1 P

0, 2, or 3

MARY

RECEIVED
SEP 25 2005
STIC

STAFF USE ONLY

Date completed: 6/20

Searcher: Mary

Terminal time:

Elapsed time:

CRU time:

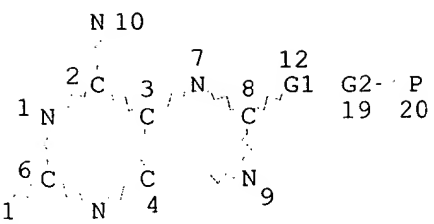
Total time: 129

Search Site
- ____ STIC
- ____ CM-1
- ____ Pre-S

Type of Search
- ____ N.A. Sequence

Vendors
- ____ IG
- 2116 STN
- ____ Dialog
- ____ APS
- ____ Geninfo

=> d l7 que stat
L5 STR



VAR G1=X/O/S/N/C
REP G2=(0-20) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L7 0 SEA FILE=REGISTRY SSS FUL L5

100.0% PROCESSED 21527 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

Searched by: Mary Hale 308-4258 CM-1 1E01

Buch
740653
Modification
7/20/02

```
=> d l10 que stat
L8                STR
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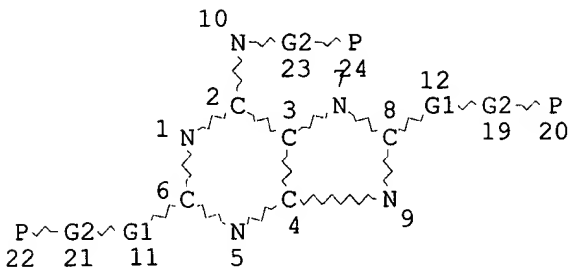


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VAR G1=X/O/S/N/C
REP G2=(0-20) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  18

STEREO ATTRIBUTES: NONE
L10           0 SEA FILE=REGISTRY SSS FUL L8

100.0% PROCESSED  26748 ITERATIONS                    0 ANSWERS
SEARCH TIME: 00.00.03


=> d l13 que stat
L11               STR
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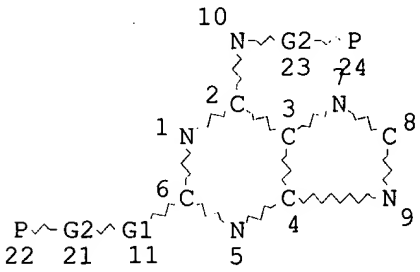


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VAR G1=X/O/S/N/C
REP G2=(0-20) A
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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
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NUMBER OF NODES IS  15

STEREO ATTRIBUTES: NONE
L13           0 SEA FILE=REGISTRY SSS FUL L11

100.0% PROCESSED  21563 ITERATIONS                    0 ANSWERS
SEARCH TIME: 00.00.03


Searched by: Mary Hale 308-4258 CM-1 1E01
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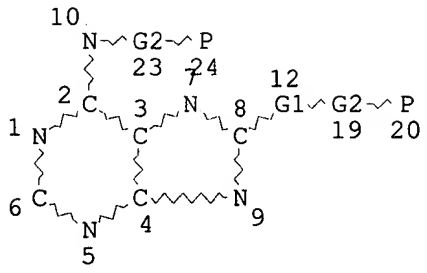
L14 STR



VAR G1=X/O/S/N/C
REP G2=(0-20) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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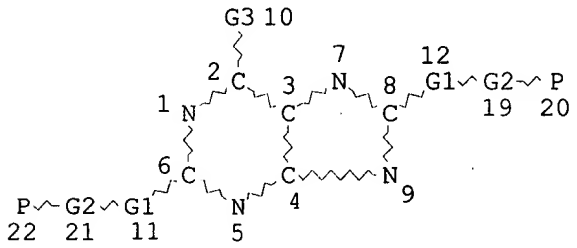
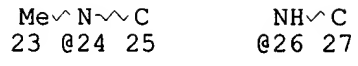
100.0% PROCESSED 28901 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

=> d l19 que stat
L17 STR





VAR G1=X/O/S/N/C
REP G2=(0-20) A
VAR G3=NH2/24/26
NODE ATTRIBUTES:
NSPEC IS RC AT 25
NSPEC IS RC AT 27
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 21

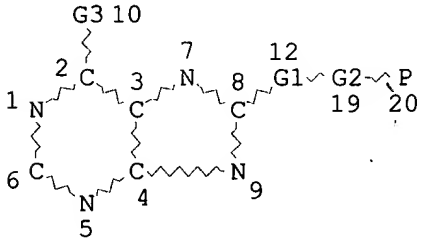
STEREO ATTRIBUTES: NONE

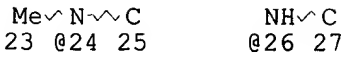
Searched by: Mary Hale 308-4258 CM-1 1E01

L19 0 SEA FILE=REGISTRY SSS FUL L17

100.0% PROCESSED 28877 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.05

=> d l23 que stat;d 1-57 ide cbib abs
L20 STR

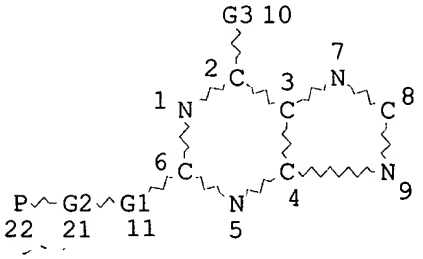


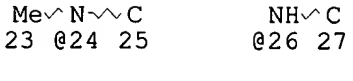


VAR G1=X/O/S/N/C
REP G2=(0-20) A
VAR G3=NH2/24/26
NODE ATTRIBUTES:
NSPEC IS RC AT 25
NSPEC IS RC AT 27
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L21 STR





VAR G1=X/O/S/N/C
REP G2=(0-20) A
VAR G3=NH2/24/26
NODE ATTRIBUTES:
NSPEC IS RC AT 25
NSPEC IS RC AT 27
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

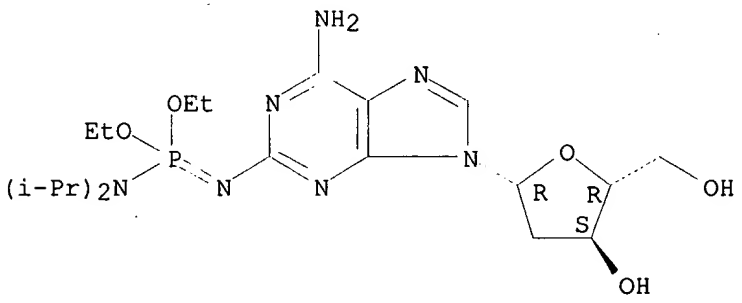
STEREO ATTRIBUTES: NONE
L23 57 SEA FILE=REGISTRY SSS FUL L20 OR L21

Searched by: Mary Hale 308-4258 CM-1 1E01

100.0% PROCESSED 28877 ITERATIONS 57 ANSWERS
SEARCH TIME: 00.00.05

L23 ANSWER 1 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 404839-85-6 REGISTRY
CN Phosphoramidimidic acid, N'-[6-amino-9-(2-deoxy-.beta.-D-erythro-pentofuranosyl)-9H-purin-2-yl]-N,N-bis(1-methylethyl)-, diethyl ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H36 N7 O5 P
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



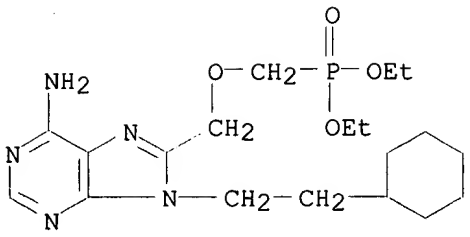
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 136:263375 Synthesis and properties of 2-azidodeoxyadenosine and its incorporation into oligodeoxynucleotides. Wada, Takeshi; Mochizuki, Akira; Higashiya, Seiichiro; Tsuruoka, Hiroyuki; Kawahara, Shun-ichi; Ishikawa, Masahide; Sekine, Mitsuo (Department of Life Science, Tokyo Institute of Technology, Midoriku, Nagatsuta, Yokohama, 226-8501, Japan). Tetrahedron Letters, 42(52), 9215-9219 (English) 2001. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..
AB 2-Azidodeoxyadenosine (I) was conveniently synthesized from deoxyguanosine by use of a combined reagent of TMSN3-BuONO. The structure of the tautomer of the azido deriv. was detd. by 1H NMR. Incorporation of I into a DNA 13mer resulted in a significant decrease of the Tm value of the DNA duplex upon hybridization with the complementary strand. The thermal stability was discussed based on the hydrogen bond energy and electrostatic repulsion.

L23 ANSWER 2 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 371778-78-8 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]methoxy]methyl]-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H32 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

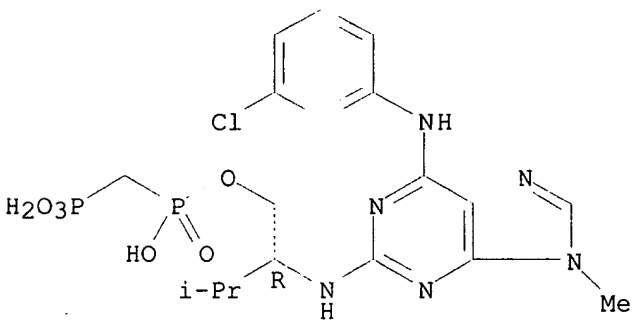
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:348869 Prodrugs phosphorus-containing compounds and pharmacodynamic action. Erion, Mark D.; Reddy, K. Raja; Robinson, Edward D.; Ugarkar, Bheemarao G. (Metabasis Therapeutics, Inc., USA). U.S. US 6312662 B1 20011106, 92 pp., Cont.-in-part of U.S. Ser. No. 263,976. (English). CODEN: USXXAM. APPLICATION: US 1999-392352 19990908. PRIORITY: US 1998-PV77164 19980306; US 1998-PV77165 19980306; US 1999-263976 19990305.

AB The present invention is directed towards novel prodrugs of phosphate, phosphonate, and phosphoramidate compds. which in their active form have a phosphate, phosphonate, or phosphoramidate group, to their prepn., to their synthetic intermediates, and to their uses. More specifically, the invention relates to the area of substituted cyclic 1,3-propanyl phosphate, phosphonate and phosphoramidate esters.

L23 ANSWER 3 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 345231-77-8 REGISTRY
CN Phosphonic acid, (phosphonomethyl)-, mono[(2R)-2-[[6-[(3-chlorophenyl)amino]-9-methyl-9H-purin-2-yl]amino]-3-methylbutyl] ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C18 H25 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



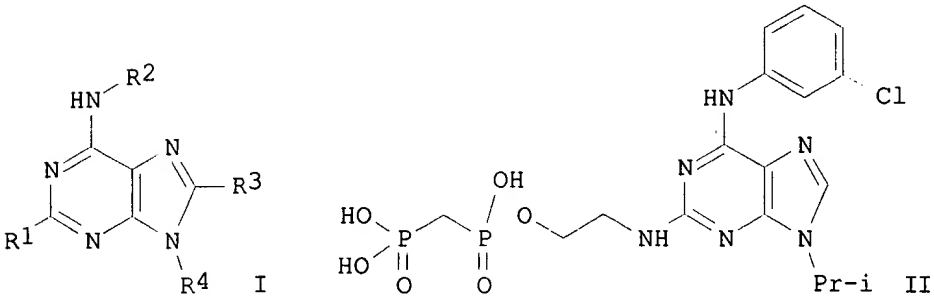
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 135:46049 Prepn. of purine derivs. for the treatment of bone related disorders and cancer. Weigele, Manfred; Shakespeare, William; Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

GI

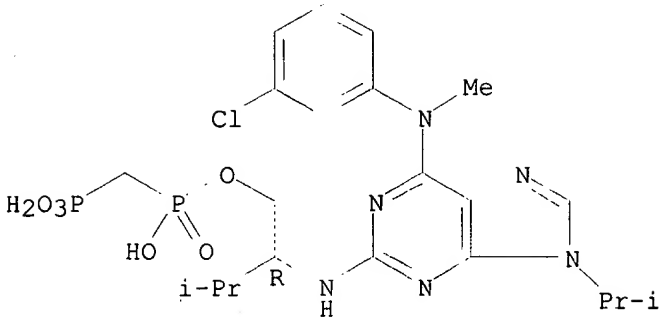


AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

L23 ANSWER 4 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 345231-76-7 REGISTRY
CN Phosphonic acid, (phosphonomethyl)-, mono[(2R)-2-[[6-[(3-chlorophenyl)methylamino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methylbutyl] ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C21 H31 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

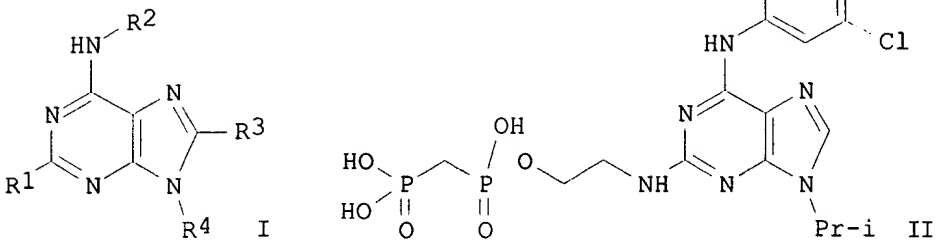


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:46049 Prepn. of purine derivs. for the treatment of bone related disorders and cancer. Weigele, Manfred; Shakespeare, William; Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

GI



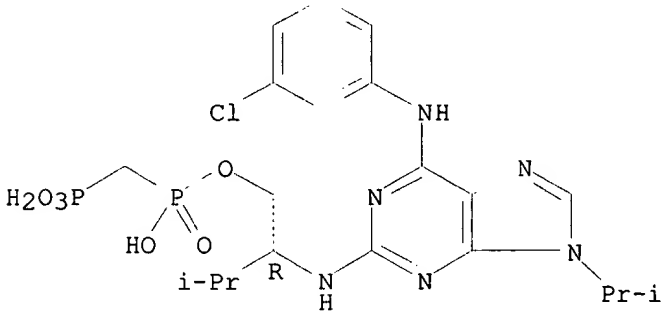
AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride).

Searched by: Mary Hale 308-4258 CM-1 1E01

The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

L23 ANSWER 5 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 345231-75-6 REGISTRY
CN Phosphonic acid, (phosphonomethyl)-, mono[(2R)-2-[[6-[(3-chlorophenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methylbutyl] ester (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C20 H29 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



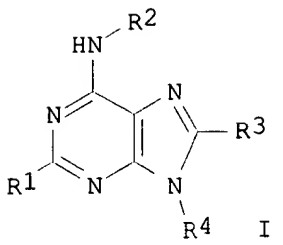
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:46049 Prepn. of purine derivs. for the treatment of bone related disorders and cancer. Weigele, Manfred; Shakespeare, William; Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



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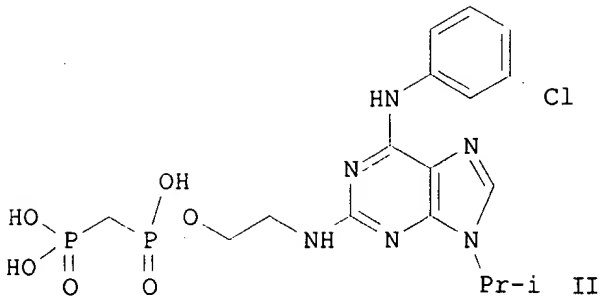

II

AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

L23 ANSWER 6 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-62-2 REGISTRY
CN Phosphonic acid, [[[3-[[6-[(3-chlorophenyl)amino]-9-[2-(3-hydroxyphenyl)ethyl]-9H-purin-2-yl]amino]propyl]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
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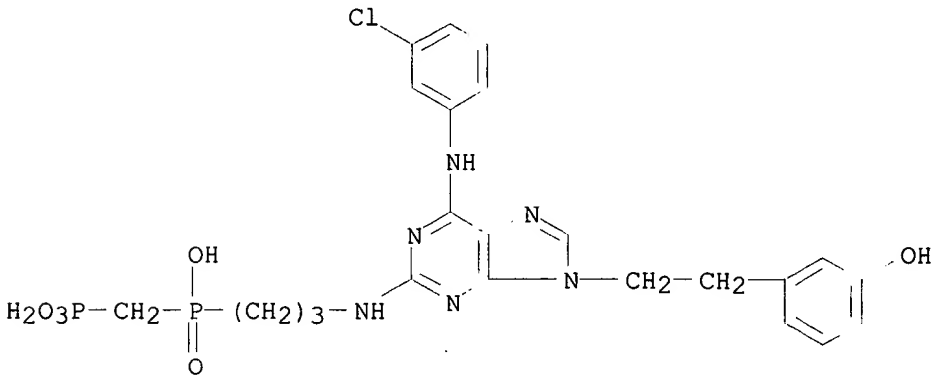

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

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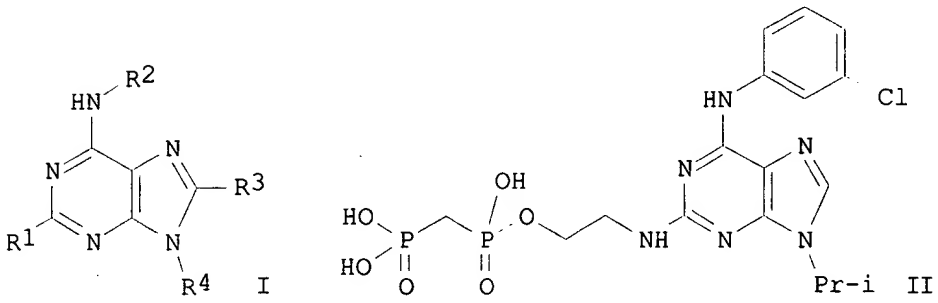

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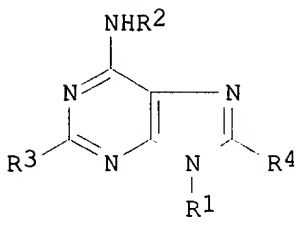

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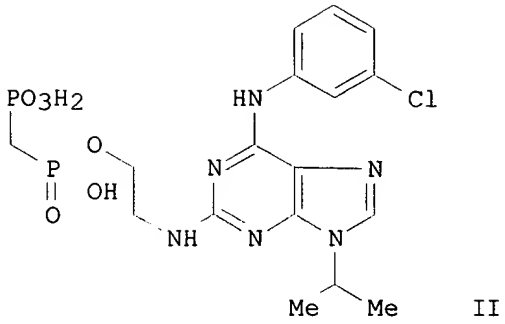

II

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

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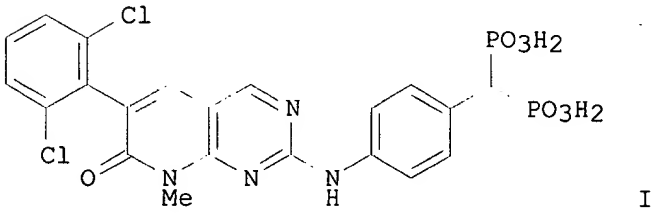

I

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl,

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L23 ANSWER 7 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-61-1 REGISTRY
CN Phosphonic acid, [[[3-[[6-[(3-chlorophenyl)amino]-9-[2-(4-hydroxyphenyl)ethyl]-9H-purin-2-yl]amino]propyl]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
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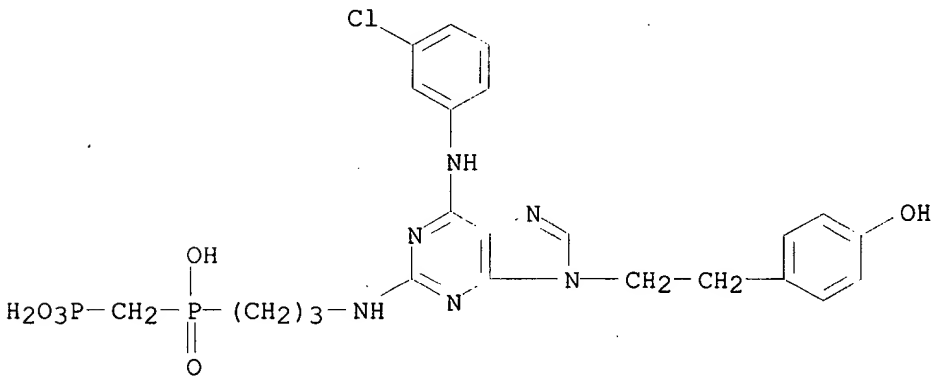
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



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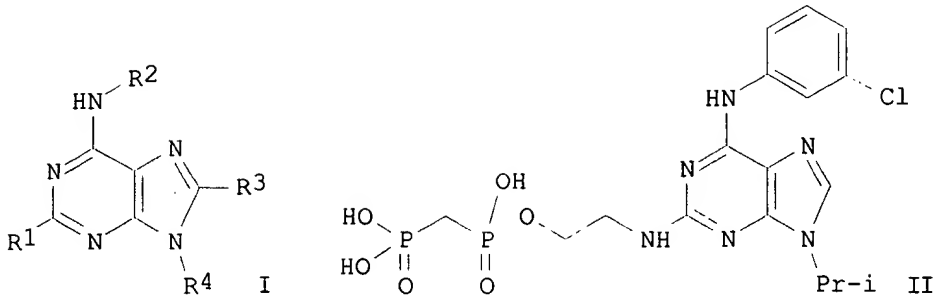

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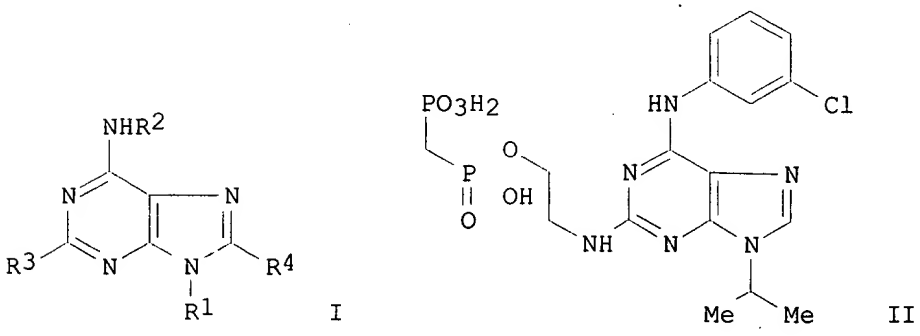

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Searched by: Mary Hale 308-4258 CM-1 1E01

heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

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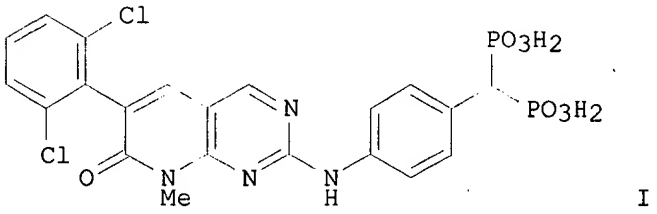

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L23 ANSWER 8 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-60-0 REGISTRY
CN Phosphonic acid, [[[3-[[6-[(3-chlorophenyl)amino]-9-[(3-hydroxyphenyl)methyl]-9H-purin-2-yl]amino]propyl]hydroxyphosphinyl]methyl]-

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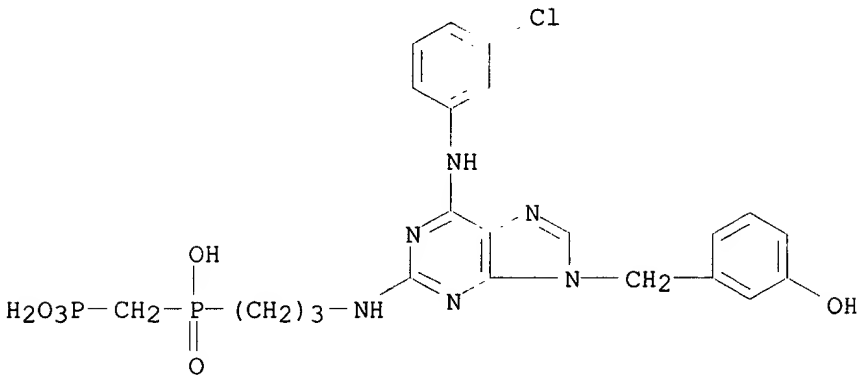

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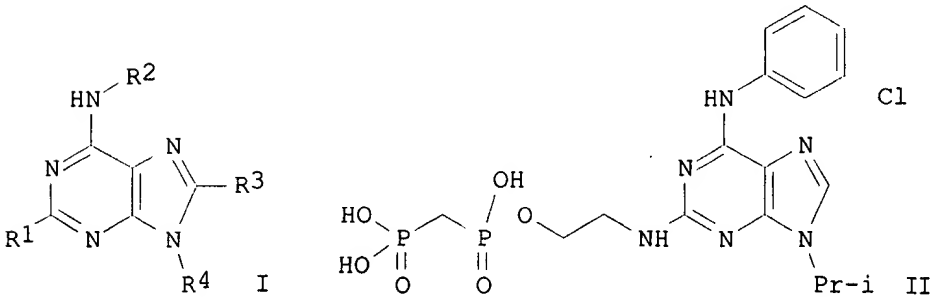

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S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

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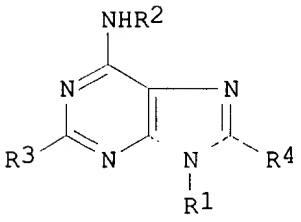
GI



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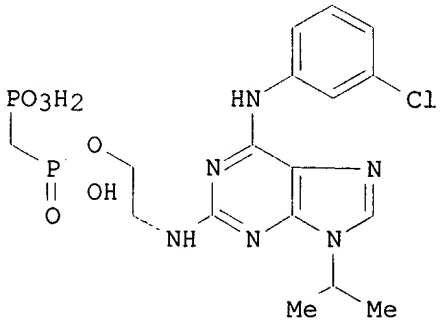

II

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

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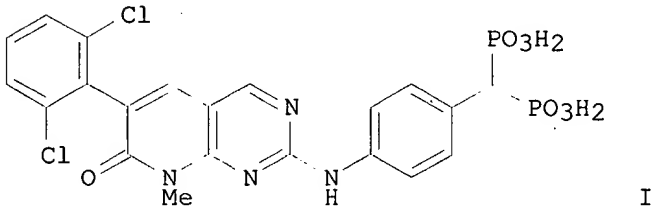

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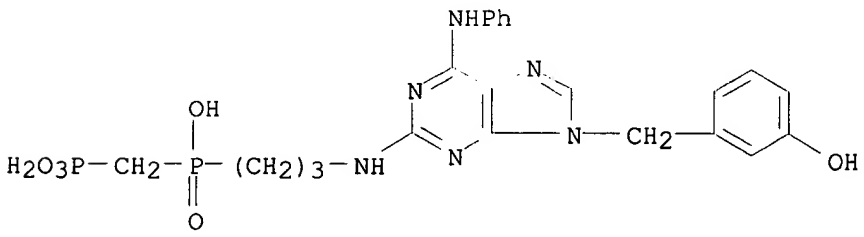
L23 ANSWER 9 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-59-7 REGISTRY
CN Phosphonic acid, [[hydroxy[3-[[9-[(3-hydroxyphenyl)methyl]-6-(phenylamino)-9H-purin-2-yl]amino]propyl]phosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C22 H26 N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



Searched by: Mary Hale 308-4258 CM-1 1E01

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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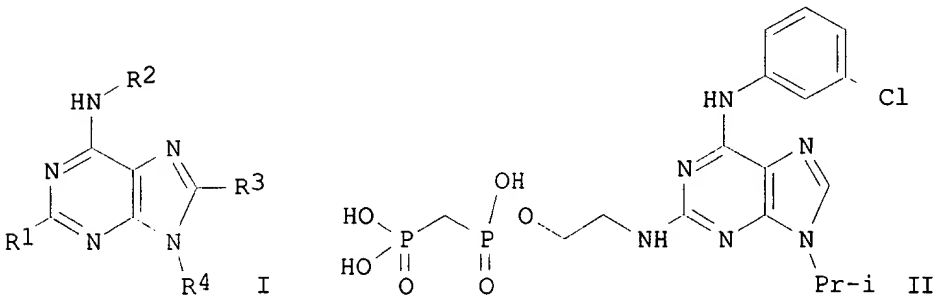
GI



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19991217; US 2000-PV240788 20001016.

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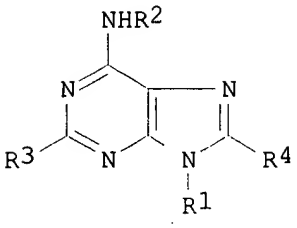

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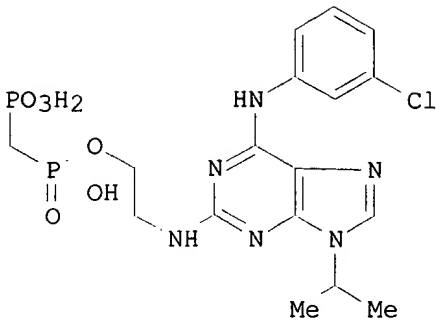

II

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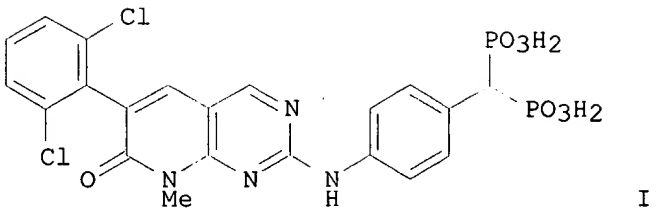

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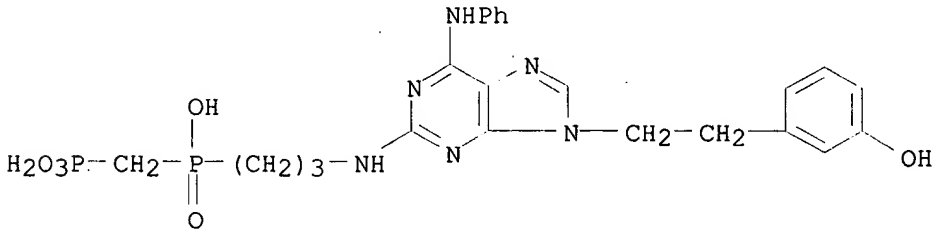
L23 ANSWER 10 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-58-6 REGISTRY
CN Phosphonic acid, [[hydroxy[3-[[9-[2-(3-hydroxyphenyl)ethyl]-6-(phenylamino)-9H-purin-2-yl]amino]propyl]phosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H28 N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



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Searched by: Mary Hale 308-4258 CM-1 1E01

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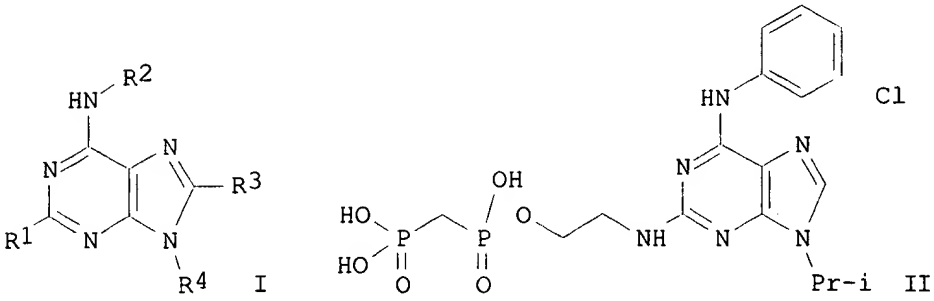

I II

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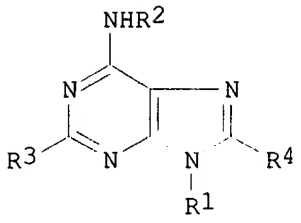

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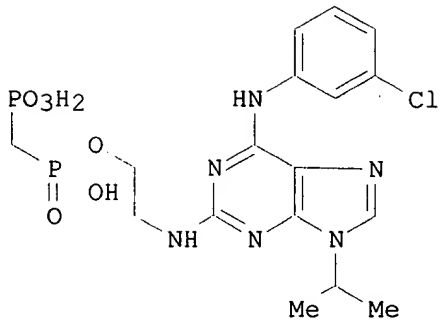

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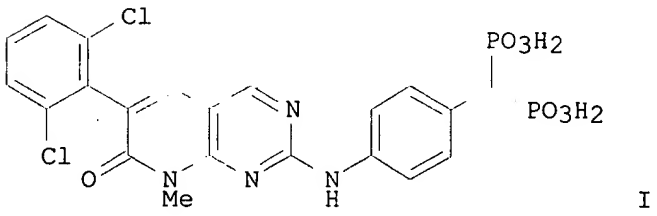

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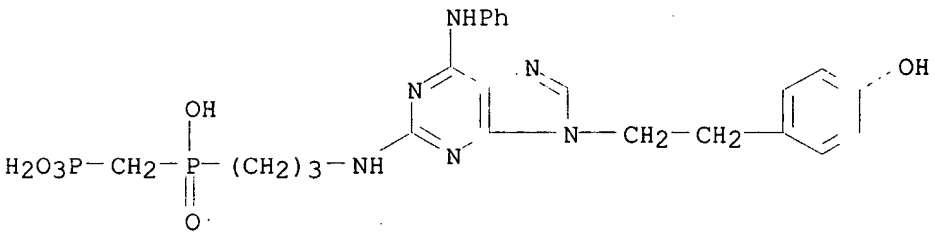
L23 ANSWER 11 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-57-5 REGISTRY
CN Phosphonic acid, [[hydroxy[3-[[9-[2-(4-hydroxyphenyl)ethyl]-6-(phenylamino)-9H-purin-2-yl]amino]propyl]phosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C23 H28 N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



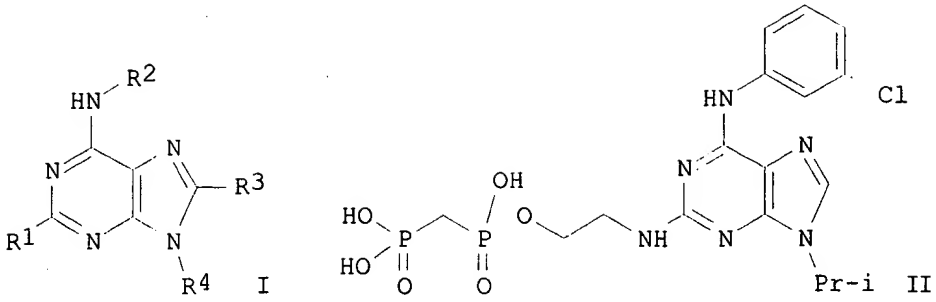
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:46049 Prepn. of purine derivs. for the treatment of bone related disorders and cancer. Weigele, Manfred; Shakespeare, William; Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

REFERENCE 2: 135:46048 Preparation of purines with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Dalgarno, David C.; Metcalf, Iii Chester A. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044259 A1 20010621, 128 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34572 20001218. PRIORITY: US 1999-PV172510 19991217; US 2000-PV240788 20001016.

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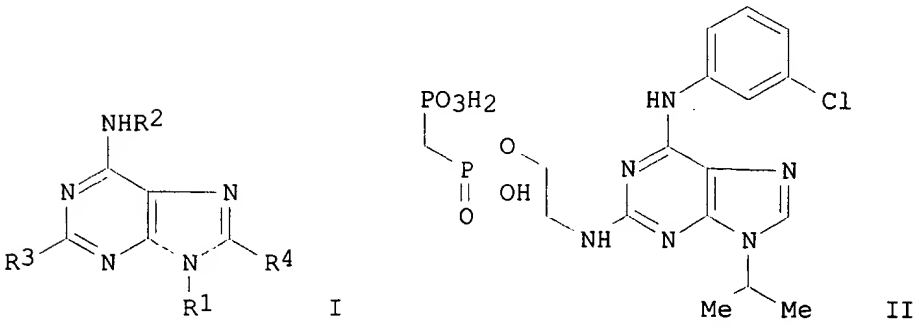

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl,

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heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

REFERENCE 3: 135:46047 Preparation of pyrimidine heterocycles with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Dalgarno, David C.; Luke, George P.; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Metcalf, Chester A., III; Vu, Chi B.; Kawahata, Noriyuki H. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044258 A1 20010621, 186 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34487 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016; US 2000-741619 20001218; US 2000-740653 20001218.

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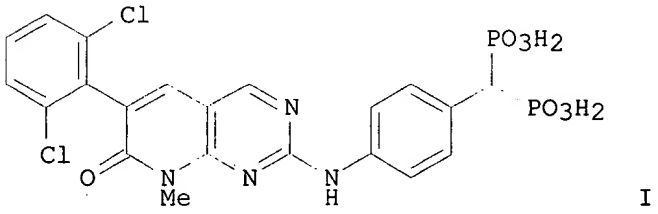

I

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl, cycloalkyl; Hc = heterocycle contg. a pyrimidine subunit; M = (CH2)n; Tb = phosphorus contg. moiety; X, Y, Z = NR, O, S; R = H, alkyl, alkenyl, aryl, heterocyclyl, heteroaryl, etc.; n = 1 - 10], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, pyrido[2,3-d]pyrimidine I was prepd. in 41% yield by condensation of Br-4-C6H4CH[P(O)(OEt)2]2 with 2-amino-6-(2,6-dichlorophenyl)-8-methyl-pyrido[2,3-d]pyrimidin-7(8H)-one using Pd(OAc)2, Cs2CO3, and (S)-BINAP in toluene. The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

L23 ANSWER 12 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-28-0 REGISTRY
CN Phosphonic acid, [[[2-[[6-[(3-chlorophenyl)amino]-9-methyl-9H-purin-2-yl]amino]-3-methylbutoxy]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)

Searched by: Mary Hale 308-4258 CM-1 1E01

FS 3D CONCORD
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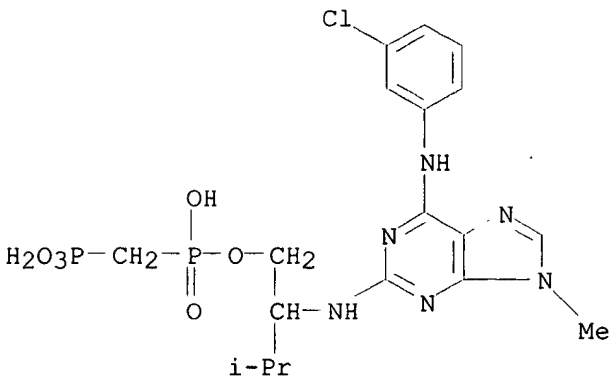
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:46048 Preparation of purines with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Dalgarno, David C.; Metcalf, Iii Chester A. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044259 A1 20010621, 128 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34572 20001218. PRIORITY: US 1999-PV172510 19991217; US 2000-PV240788 20001016.

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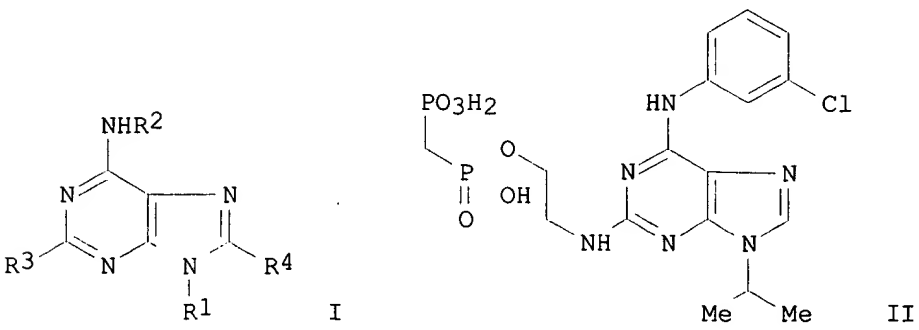

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl,

Searched by: Mary Hale 308-4258 CM-1 1E01

aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

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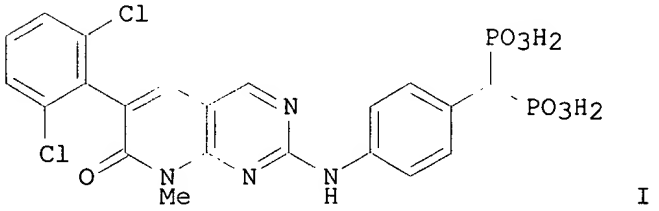


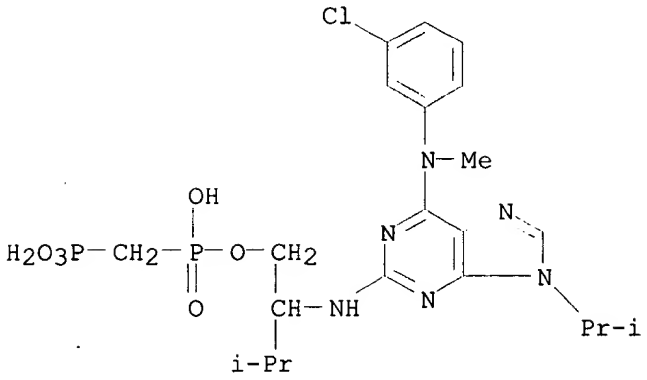
I

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl, cycloalkyl; Hc = heterocycle contg. a pyrimidine subunit; M = (CH2)n; Tb = phosphorus contg. moiety; X, Y, Z = NR, O, S; R = H, alkyl, alkenyl, aryl, heterocyclyl, heteroaryl, etc.; n = 1 - 10], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, pyrido[2,3-d]pyrimidine I was prepd. in 41% yield by condensation of Br-4-C6H4CH[P(O)(OEt)2]2 with 2-amino-6-(2,6-dichlorophenyl)-8-methyl-pyrido[2,3-d]pyrimidin-7(8H)-one using Pd(OAc)2, Cs2CO3, and (S)-BINAP in toluene. The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

L23 ANSWER 13 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-27-9 REGISTRY
CN Phosphonic acid, [[[2-[[6-[(3-chlorophenyl)methylamino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methylbutoxy]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H31 Cl N6 O6 P2

Searched by: Mary Hale 308-4258 CM-1 1E01

SR CA
LC STN Files: CA, CAPLUS, USPATFULL



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2 REFERENCES IN FILE CA (1967 TO DATE)
2 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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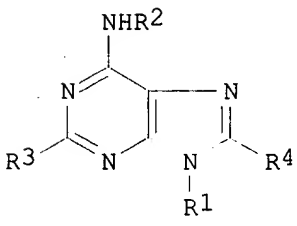

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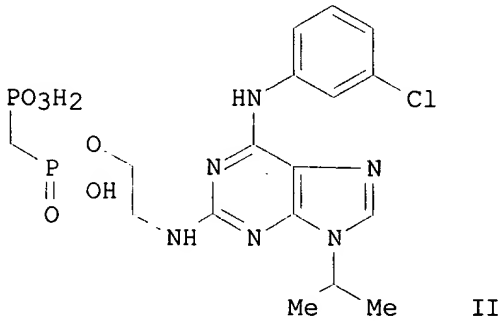

II

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease,

Searched by: Mary Hale 308-4258 CM-1 1E01

hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

REFERENCE 2: 135:46047 Preparation of pyrimidine heterocycles with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Dalgarno, David C.; Luke, George P.; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Metcalf, Chester A., III; Vu, Chi B.; Kawahata, Noriyuki H. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044258 A1 20010621, 186 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34487 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016; US 2000-741619 20001218; US 2000-740653 20001218.

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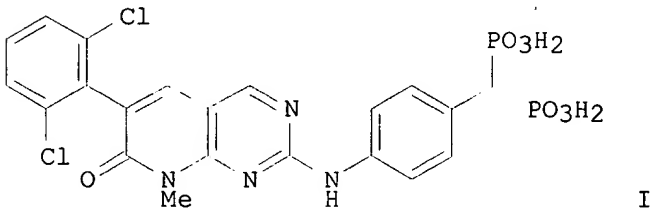
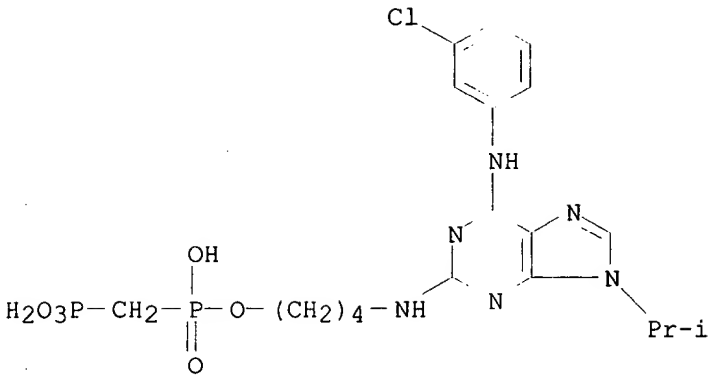


I

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl, cycloalkyl; Hc = heterocycle contg. a pyrimidine subunit; M = (CH2)n; Tb = phosphorus contg. moiety; X, Y, Z = NR, O, S; R = H, alkyl, alkenyl, aryl, heterocyclyl, heteroaryl, etc.; n = 1 - 10], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, pyrido[2,3-d]pyrimidine I was prepd. in 41% yield by condensation of Br-4-C6H4CH[P(O)(OEt)2]2 with 2-amino-6-(2,6-dichlorophenyl)-8-methyl-pyrido[2,3-d]pyrimidin-7(8H)-one using Pd(OAc)2, Cs2CO3, and (S)-BINAP in toluene. The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

L23 ANSWER 14 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-26-8 REGISTRY
CN Phosphonic acid, [[[4-[[6-[(3-chlorophenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]butoxy]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H27 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

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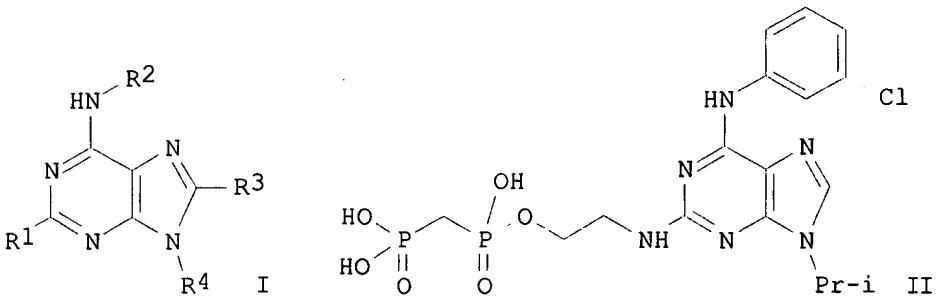

AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol,

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3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

REFERENCE 2: 135:46048 Preparation of purines with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Dalgarno, David C.; Metcalf, Iii Chester A. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044259 A1 20010621, 128 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34572 20001218. PRIORITY: US 1999-PV172510 19991217; US 2000-PV240788 20001016.

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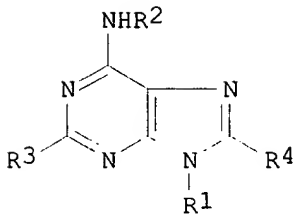

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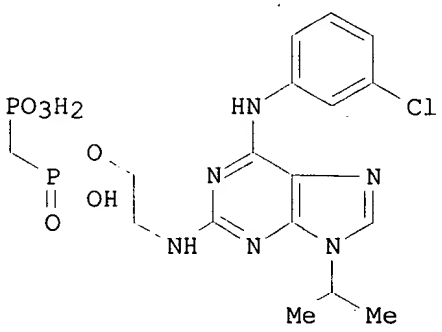

II

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

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UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34487 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016; US 2000-741619 20001218; US 2000-740653 20001218.

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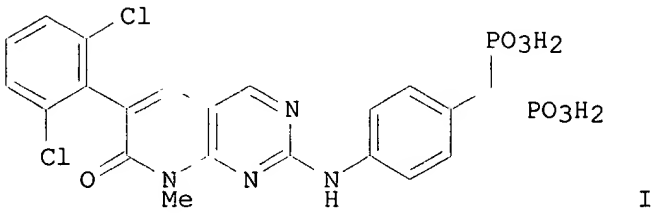
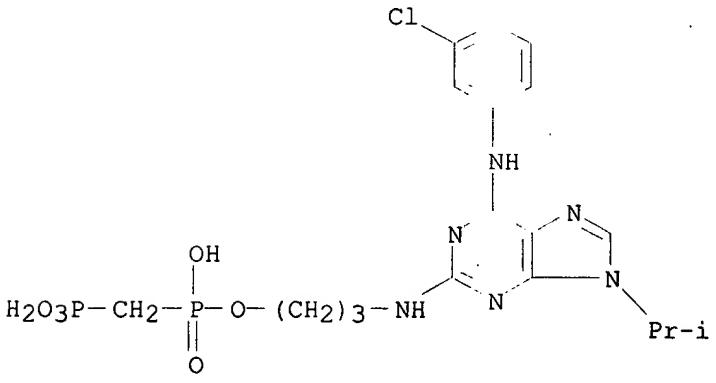


I

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl, cycloalkyl; Hc = heterocycle contg. a pyrimidine subunit; M = (CH2)n; Tb = phosphorus contg. moiety; X, Y, Z = NR, O, S; R = H, alkyl, alkenyl, aryl, heterocyclyl, heteroaryl, etc.; n = 1 - 10], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, pyrido[2,3-d]pyrimidine I was prepd. in 41% yield by condensation of Br-4-C6H4CH[P(O)(OEt)2]2 with 2-amino-6-(2,6-dichlorophenyl)-8-methyl-pyrido[2,3-d]pyrimidin-7(8H)-one using Pd(OAc)2, Cs2CO3, and (S)-BINAP in toluene. The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

L23 ANSWER 15 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-25-7 REGISTRY
CN Phosphonic acid, [[[3-[[6-[(3-chlorophenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]propoxy]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H25 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 1E01

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:46049 Prepn. of purine derivs. for the treatment of bone related disorders and cancer. Weigele, Manfred; Shakespeare, William; Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

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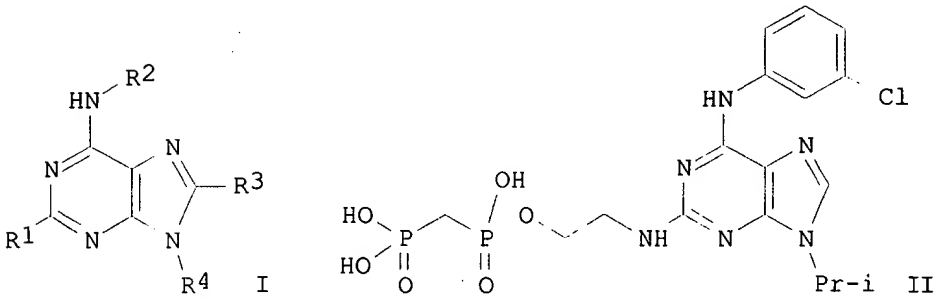

AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

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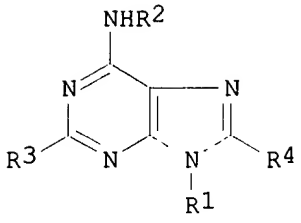

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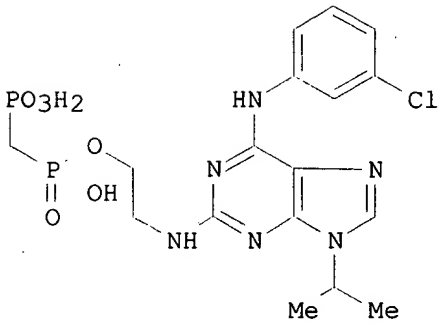

II

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

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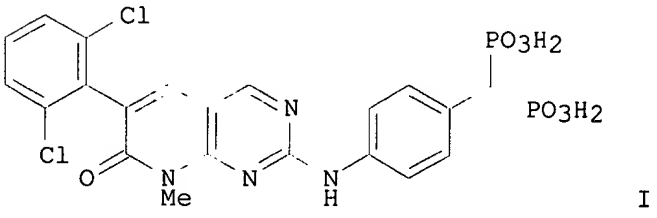

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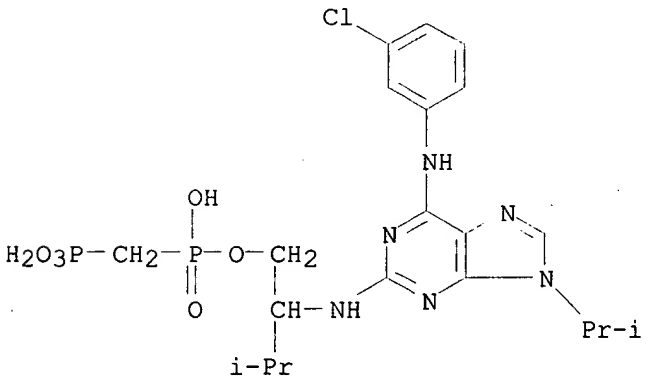
Searched by: Mary Hale 308-4258 CM-1 1E01

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl, cycloalkyl; Hc = heterocycle contg. a pyrimidine subunit; M = (CH2)n; Tb = phosphorus contg. moiety; X, Y, Z = NR, O, S; R = H, alkyl, alkenyl, aryl, heterocyclyl, heteroaryl, etc.; n = 1 - 10], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, pyrido[2,3-d]pyrimidine I was prepd. in 41% yield by condensation of Br-4-C6H4CH[P(O)(OEt)2]2 with 2-amino-6-(2,6-dichlorophenyl)-8-methyl-pyrido[2,3-d]pyrimidin-7(8H)-one using Pd(OAc)2, Cs2CO3, and (S)-BINAP in toluene. The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

L23 ANSWER 16 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-24-6 REGISTRY
CN Phosphonic acid, [[[2-[[6-[(3-chlorophenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]-3-methylbutoxy]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C20 H29 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



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2 REFERENCES IN FILE CA (1967 TO DATE)
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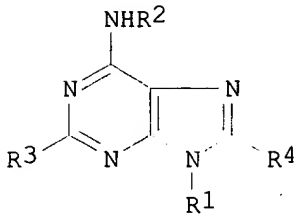

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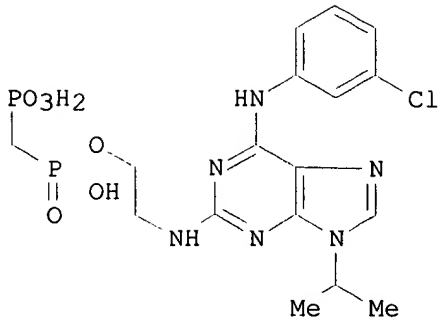

II

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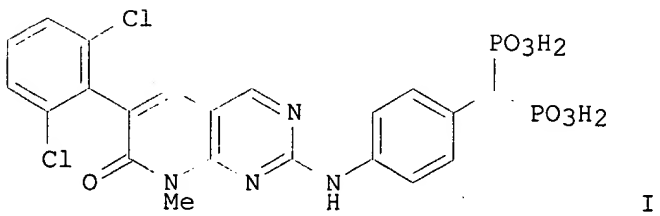

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Searched by: Mary Hale 308-4258 CM-1 1E01

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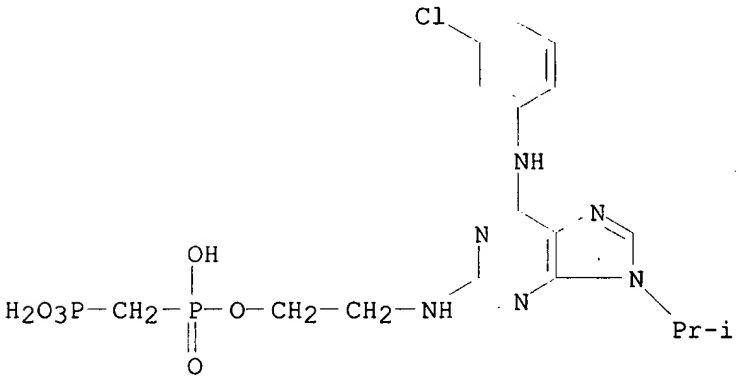
L23 ANSWER 17 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 344585-23-5 REGISTRY
CN Phosphonic acid, [[[2-[[6-[(3-chlorophenyl)amino]-9-(1-methylethyl)-9H-purin-2-yl]amino]ethoxy]hydroxyphosphinyl]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C17 H23 Cl N6 O6 P2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



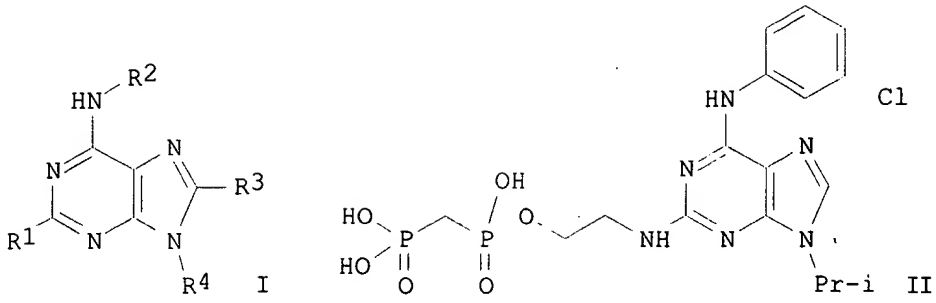
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:46049 Prepn. of purine derivs. for the treatment of bone related disorders and cancer. Weigele, Manfred; Shakespeare, William; Sawyer, Tomi K.; Sundaramoorthi, Rajeswari; Bohacek, Regine; Wang, Yihan; Metcalf, Chester A., III (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044260 A2 20010621, 168 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34417 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016.

GI

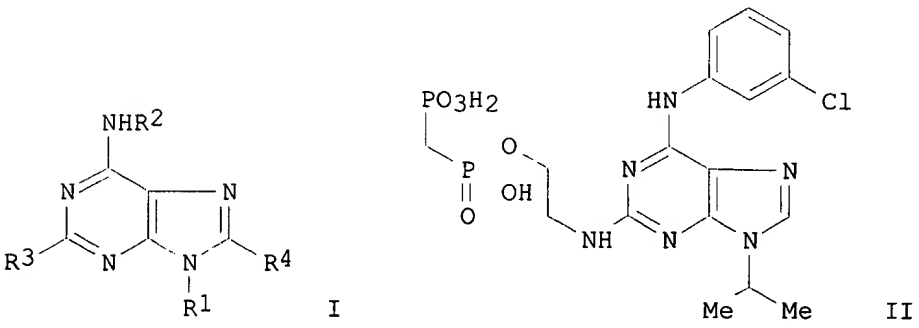
Searched by: Mary Hale 308-4258 CM-1 1E01



AB Purine derivs., such as I [R1, R3 = H, halogen, Y (Y = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl), ZR5 {Z = O, S, NR6; (R5, R6 = aliph., heteroaliph., aryl, heteroaryl, alkylaryl, alkylheteroaryl)}; R2 = Y; R4 = H, Y; whereby at least one of the R1, R2, R3 or R4 as defined above, is substituted by one or more phosphorus moieties] were prepd. for the treatment of bone related disorders and cancer. Thus, purine deriv. II was prepd. via multistep synthetic sequence starting from 6-chloro-2-fluoro-9H-purine, 2-propanol, 3-chloroaniline, ethanolamine and methylenebis(phosphonic dichloride). The prepd. purine derivs. were tested for their ability to inhibit protein kinases, to bind to bone, to inhibit bone resorption or to otherwise improve the relative dynamics of bone homeostasis.

REFERENCE 2: 135:46048 Preparation of purines with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Dalgarno, David C.; Metcalf, Iii Chester A. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044259 A1 20010621, 128 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, HU, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU; RW: AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34572 20001218. PRIORITY: US 1999-PV172510 19991217; US 2000-PV240788 20001016.

GI



Searched by: Mary Hale 308-4258 CM-1 1E01

AB Purines with a phosphorus contg. moiety, such as I [R1 = H, alkyl, heteroalkyl, aryl, heteroaryl; R2 = phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R3 = H, halogen, phosphorus moiety contg. alkyl, heteroalkyl, aryl, heteroaryl; R4 = H, halogen, alkyl, heteroalkyl, aryl, heteroaryl], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, purine II via a five step synthetic sequence starting from 2-amino-6-chloropurine 2-propanol, 3-chloroaniline, 2-aminoethanol, and methylenebis(phosphonic dichloride). The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

REFERENCE 3: 135:46047 Preparation of pyrimidine heterocycles with a phosphorus containing moiety for pharmaceutical use in the treatment of bone disorders. Weigele, Manfred; Dalgarno, David C.; Luke, George P.; Sawyer, Tomi K.; Bohacek, Regine; Shakespeare, William C.; Sundaramoorthi, Rajeswari; Wang, Yihan; Metcalf, Chester A., III; Vu, Chi B.; Kawahata, Noriyuki H. (Ariad Pharmaceuticals, Inc., USA). PCT Int. Appl. WO 2001044258 A1 20010621, 186 pp. DESIGNATED STATES: W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG, TR. (English). CODEN: PIXXD2. APPLICATION: WO 2000-US34487 20001218. PRIORITY: US 1999-PV172510 19991217; US 1999-PV172161 19991217; US 2000-PV240788 20001016; US 2000-741619 20001218; US 2000-740653 20001218.

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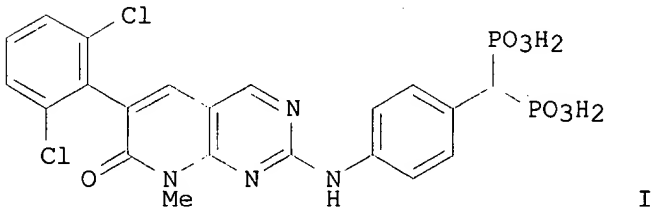


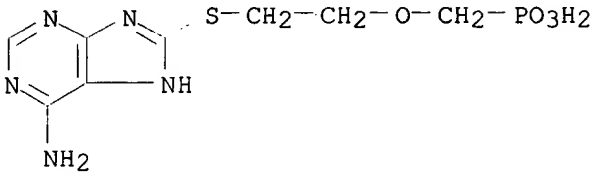
I

AB Heterocycles with a pyrimidine subunit and a phosphorus contg. moiety, such as Hc-X-M-Y-M-Cy-M-Y-M-Z-Tb [Cy = aryl, heterocyclyl, heteroaryl, cycloalkyl; Hc = heterocycle contg. a pyrimidine subunit; M = (CH2)n; Tb = phosphorus contg. moiety; X, Y, Z = NR, O, S; R = H, alkyl, alkenyl, aryl, heterocyclyl, heteroaryl, etc.; n = 1 - 10], were prepd. for pharmaceutical use in the treatment of debilitating bone disorders, such as osteoporosis, Paget's disease, hyperparathyroidism, various cancers where bone tissue resorption is increased, and rheumatoid arthritis. Thus, pyrido[2,3-d]pyrimidine I was prepd. in 41% yield by condensation of Br-4-C6H4CH[P(O)(OEt)2]2 with 2-amino-6-(2,6-dichlorophenyl)-8-methyl-pyrido[2,3-d]pyrimidin-7(8H)-one using Pd(OAc)2, Cs2CO3, and (S)-BINAP in toluene. The prepd. phosphorus contg. purines were tested for anti-resorption activity, Src kinase inhibition, and inhibition of tumor growth.

L23 ANSWER 18 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328381-19-7 REGISTRY
CN Phosphonic acid, [[2-[(6-amino-1H-purin-8-yl)thio]ethoxy]methyl]- (9CI)

Searched by: Mary Hale 308-4258 CM-1 1E01

(CA INDEX NAME)
FS 3D CONCORD
MF C8 H12 N5 O4 P S
SR CA
LC STN Files: CA, CAPLUS, CASREACT



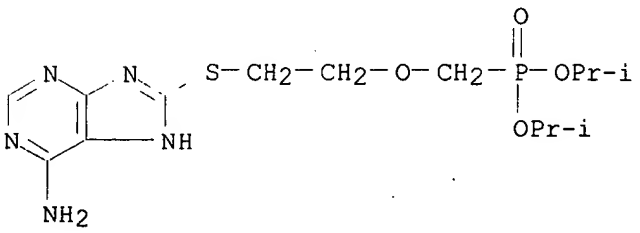
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208047 Synthesis of acyclic nucleoside and nucleotide analogs derived from 6-amino-7H-purine-8(9H)-thione and 8-(methylsulfanyl)adenine. Janeba, Zlatko; Holy, Antonin; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1698-1712 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Reaction of 8-bromoadenine derivs. with thiourea in ethanol or butanol was used for the synthesis of the corresponding N9-substituted 6-amino-7H-purine-8(9H)-thiones. 8-(Methylsulfanyl)adenine derivs. were prepd. by reaction of thiones with iodomethane in 1 M sodium methoxide or in aq. 1.5 M potassium hydroxide. Alkylation of 6-amino-7H-purine-8(9H)-thione proceeds preferentially on the sulfur atom. Under similar conditions, alkylation of 8-(methylsulfanyl)adenine with diverse alkylation agents afforded N9-substituted adenine derivs. and N3-substituted adenine derivs. 8,3'-S-Anhydro nucleosides were prepd. in good yields by cyclization of 6-amino-7H-purine-8(9H)-thiones under the Mitsunobu reaction conditions.

L23 ANSWER 19 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328381-18-6 REGISTRY
CN Phosphonic acid, [[2-[(6-amino-1H-purin-8-yl)thio]ethoxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H24 N5 O4 P S
SR CA
LC STN Files: CA, CAPLUS, CASREACT



Searched by: Mary Hale 308-4258 CM-1 1E01

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208047 Synthesis of acyclic nucleoside and nucleotide analogs derived from 6-amino-7H-purine-8(9H)-thione and 8-(methylsulfanyl)adenine. Janeba, Zlatko; Holy, Antonin; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1698-1712 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Reaction of 8-bromoadenine derivs. with thiourea in ethanol or butanol was used for the synthesis of the corresponding N9-substituted 6-amino-7H-purine-8(9H)-thiones. 8-(Methylsulfanyl)adenine derivs. were prepd. by reaction of thiones with iodomethane in 1 M sodium methoxide or in aq. 1.5 M potassium hydroxide. Alkylation of 6-amino-7H-purine-8(9H)-thione proceeds preferentially on the sulfur atom. Under similar conditions, alkylation of 8-(methylsulfanyl)adenine with diverse alkylation agents afforded N9-substituted adenine derivs. and N3-substituted adenine derivs. 8,3'-S-Anhydro nucleosides were prepd. in good yields by cyclization of 6-amino-7H-purine-8(9H)-thiones under the Mitsunobu reaction conditions.

L23 ANSWER 20 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328378-83-2 REGISTRY
CN Phosphonic acid, [[1-[[(6-amino-1H-purin-2-yl)oxy]methyl]-2-(triphenylmethoxy)ethoxy]methyl]- (9CI) (CA INDEX NAME)
MF C28 H28 N5 O6 P
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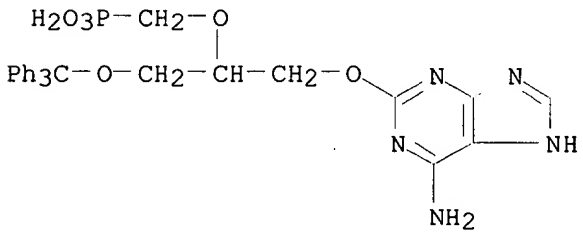
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208048 Synthesis of acyclic nucleotide analogs derived from N3-substituted isoguanine. Alexander, Petr; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1713-1725 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Reaction of 9-benzyl-6-{[(dimethylamino)methylidene]amino}purin-2(3H)-one (I) with ethylene carbonate gave a mixt. of 9-benzyl-2-(2-hydroxyethoxy)purin-6-amine and 2-amino-9-benzyl-3-(2-hydroxyethyl)purin-2(3H)-one. This mixt. reacted with diisopropyl

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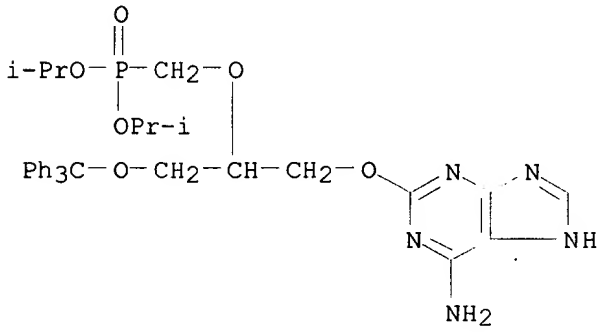
(tosyloxymethyl)phosphonate in the presence of NaH followed by catalytic hydrogenation and bromotrimethylsilane treatment to afford isomeric 6-amino-3-[2-(phosphonomethoxy)ethyl]purin-2(3H)-one (II) and 2-[2-(phosphonomethoxy)ethoxy]purin-6-amine (III). Similar treatment of compd. I with tritylglycidol gave two isomeric 2-hydroxy-3-(trityloxy)propyl deriv. diisopropyl (tosyloxymethyl)phosphonate to afford protected diester intermediates. These compds. were transformed by hydrogenolysis and ester cleavage with bromotrimethylsilane to the isomeric 6-amino-3-[3-hydroxy-2-(phosphonomethoxy)propyl]-purin-2(3H)-one (IV) and 2-[3-hydroxy-2-(phosphonomethoxy)propoxy]purin-6-amine (V). None of the free phosphonates II-V exhibited any antiviral or cytostatic activity.

L23 ANSWER 21 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328378-82-1 REGISTRY
CN Phosphonic acid, [[1-[[(6-amino-1H-purin-2-yl)oxy]methyl]-2-(triphenylmethoxy)ethoxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
MF C34 H40 N5 O6 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208048 Synthesis of acyclic nucleotide analogs derived from N3-substituted isoguanine. Alexander, Petr; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1713-1725 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Reaction of 9-benzyl-6-{[(dimethylamino)methylidene]amino}purin-2(3H)-one (I) with ethylene carbonate gave a mixt. of 9-benzyl-2-(2-hydroxyethoxy)purin-6-amine and 2-amino-9-benzyl-3-(2-hydroxyethyl)purin-2(3H)-one. This mixt. reacted with diisopropyl (tosyloxymethyl)phosphonate in the presence of NaH followed by catalytic hydrogenation and bromotrimethylsilane treatment to afford isomeric 6-amino-3-[2-(phosphonomethoxy)ethyl]purin-2(3H)-one (II) and 2-[2-(phosphonomethoxy)ethoxy]purin-6-amine (III). Similar treatment of compd. I with tritylglycidol gave two isomeric 2-hydroxy-3-(trityloxy)propyl deriv. diisopropyl (tosyloxymethyl)phosphonate to afford protected diester intermediates. These compds. were transformed by

Searched by: Mary Hale 308-4258 CM-1 1E01

hydrogenolysis and ester cleavage with bromotrimethylsilane to the isomeric 6-amino-3-[3-hydroxy-2-(phosphonomethoxy)propyl]-purin-2(3H)-one (IV) and 2-[3-hydroxy-2-(phosphonomethoxy)propoxy]purin-6-amine (V). None of the free phosphonates II-V exhibited any antiviral or cytostatic activity.

L23 ANSWER 22 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328378-80-9 REGISTRY
CN Phosphonic acid, [[1-[[[6-amino-9-(phenylmethyl)-9H-purin-2-yl]oxy]methyl]-2-(triphenylmethoxy)ethoxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
MF C41 H46 N5 O6 P
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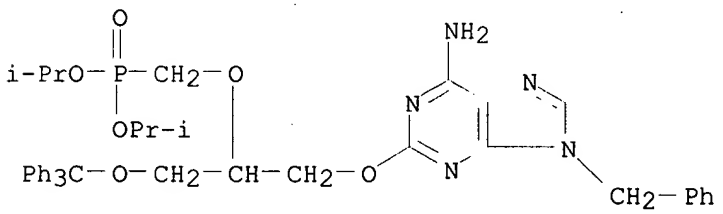
LC STN Files: CA, CAPLUS, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

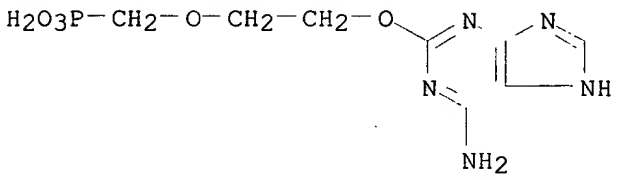
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208048 Synthesis of acyclic nucleotide analogs derived from N3-substituted isoguanine. Alexander, Petr; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1713-1725 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.
AB Reaction of 9-benzyl-6-{[(dimethylamino)methylidene]amino}purin-2(3H)-one (I) with ethylene carbonate gave a mixt. of 9-benzyl-2-(2-hydroxyethoxy)purin-6-amine and 2-amino-9-benzyl-3-(2-hydroxyethyl)purin-2(3H)-one. This mixt. reacted with diisopropyl (tosyloxymethyl)phosphonate in the presence of NaH followed by catalytic hydrogenation and bromotrimethylsilane treatment to afford isomeric 6-amino-3-[2-(phosphonomethoxy)ethyl]purin-2(3H)-one (II) and 2-[2-(phosphonomethoxy)ethoxy]purin-6-amine (III). Similar treatment of compd. I with tritylglycidol gave two isomeric 2-hydroxy-3-(trityloxy)propyl deriv. diisopropyl (tosyloxymethyl)phosphonate to afford protected diester intermediates. These compds. were transformed by hydrogenolysis and ester cleavage with bromotrimethylsilane to the isomeric 6-amino-3-[3-hydroxy-2-(phosphonomethoxy)propyl]-purin-2(3H)-one (IV) and 2-[3-hydroxy-2-(phosphonomethoxy)propoxy]purin-6-amine (V). None of the free phosphonates II-V exhibited any antiviral or cytostatic activity.

L23 ANSWER 23 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328378-75-2 REGISTRY
CN Phosphonic acid, [[2-[(6-amino-1H-purin-2-yl)oxy]ethoxy]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD

Searched by: Mary Hale 308-4258 CM-1 1E01

MF C8 H12 N5 O5 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

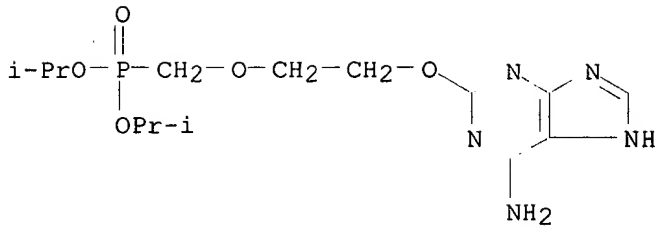
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208048 Synthesis of acyclic nucleotide analogs derived from N3-substituted isoguanine. Alexander, Petr; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1713-1725 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Reaction of 9-benzyl-6-{[(dimethylamino)methylidene]amino}purin-2(3H)-one (I) with ethylene carbonate gave a mixt. of 9-benzyl-2-(2-hydroxyethoxy)purin-6-amine and 2-amino-9-benzyl-3-(2-hydroxyethyl)purin-2(3H)-one. This mixt. reacted with diisopropyl (tosyloxymethyl)phosphonate in the presence of NaH followed by catalytic hydrogenation and bromotrimethylsilane treatment to afford isomeric 6-amino-3-[2-(phosphonomethoxy)ethyl]purin-2(3H)-one (II) and 2-[2-(phosphonomethoxy)ethoxy]purin-6-amine (III). Similar treatment of compd. I with tritylglycidol gave two isomeric 2-hydroxy-3-(trityloxy)propyl deriv. diisopropyl (tosyloxymethyl)phosphonate to afford protected diester intermediates. These compds. were transformed by hydrogenolysis and ester cleavage with bromotrimethylsilane to the isomeric 6-amino-3-[3-hydroxy-2-(phosphonomethoxy)propyl]-purin-2(3H)-one (IV) and 2-[3-hydroxy-2-(phosphonomethoxy)propoxy]purin-6-amine (V). None of the free phosphonates II-V exhibited any antiviral or cytostatic activity.

L23 ANSWER 24 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328378-74-1 REGISTRY
CN Phosphonic acid, [[2-[(6-amino-1H-purin-2-yl)oxy]ethoxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H24 N5 O5 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER

Searched by: Mary Hale 308-4258 CM-1 1E01



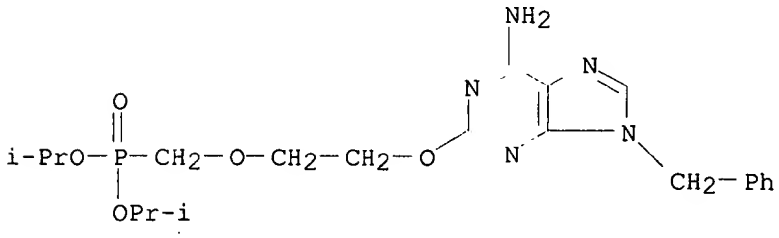
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208048 Synthesis of acyclic nucleotide analogs derived from N3-substituted isoguanine. Alexander, Petr; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1713-1725 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

AB Reaction of 9-benzyl-6-{[(dimethylamino)methylidene]amino}purin-2(3H)-one (I) with ethylene carbonate gave a mixt. of 9-benzyl-2-(2-hydroxyethoxy)purin-6-amine and 2-amino-9-benzyl-3-(2-hydroxyethyl)purin-2(3H)-one. This mixt. reacted with diisopropyl (tosyloxymethyl)phosphonate in the presence of NaH followed by catalytic hydrogenation and bromotrimethylsilane treatment to afford isomeric 6-amino-3-[2-(phosphonomethoxy)ethyl]purin-2(3H)-one (II) and 2-[2-(phosphonomethoxy)ethoxy]purin-6-amine (III). Similar treatment of compd. I with tritylglycidol gave two isomeric 2-hydroxy-3-(trityloxy)propyl deriv. diisopropyl (tosyloxymethyl)phosphonate to afford protected diester intermediates. These compds. were transformed by hydrogenolysis and ester cleavage with bromotrimethylsilane to the isomeric 6-amino-3-[3-hydroxy-2-(phosphonomethoxy)propyl]-purin-2(3H)-one (IV) and 2-[3-hydroxy-2-(phosphonomethoxy)propoxy]purin-6-amine (V). None of the free phosphonates II-V exhibited any antiviral or cytostatic activity.

L23 ANSWER 25 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 328378-72-9 REGISTRY
CN Phosphonic acid, [[2-[[6-amino-9-(phenylmethyl)-9H-purin-2-yl]oxy]ethoxy]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C21 H30 N5 O5 P
SR CA
LC STN Files: CA, CAPLUS, CASREACT, TOXCENTER



Searched by: Mary Hale 308-4258 CM-1 1E01

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 134:208048 Synthesis of acyclic nucleotide analogs derived from N3-substituted isoguanine. Alexander, Petr; Holy, Antonin; Budesinsky, Milos; Masojidkova, Milena (Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic, Prague, 16610/6, Czech Rep.). Collection of Czechoslovak Chemical Communications, 65(11), 1713-1725 (English) 2000. CODEN: CCCCAK. ISSN: 0010-0765. Publisher: Institute of Organic Chemistry and Biochemistry, Academy of Sciences of the Czech Republic.

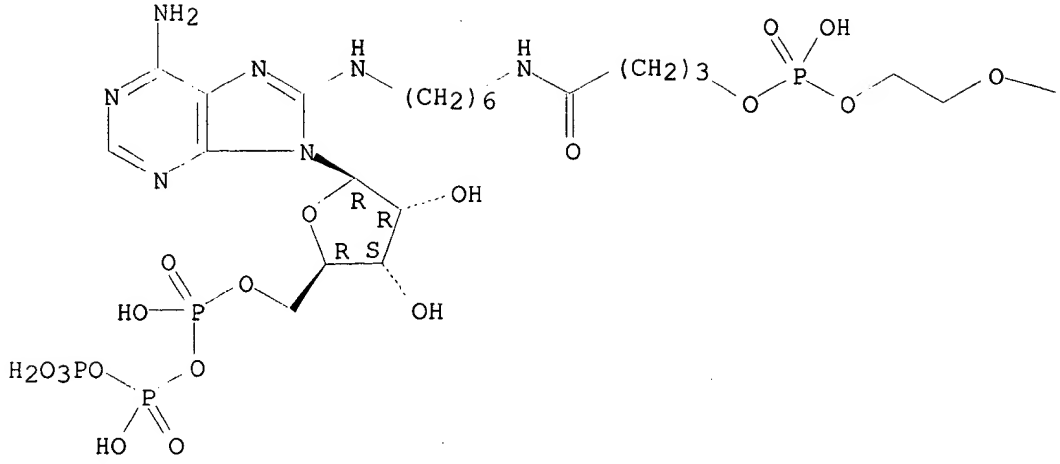
AB Reaction of 9-benzyl-6-{[(dimethylamino)methylidene]amino}purin-2(3H)-one (I) with ethylene carbonate gave a mixt. of 9-benzyl-2-(2-hydroxyethoxy)purin-6-amine and 2-amino-9-benzyl-3-(2-hydroxyethyl)purin-2(3H)-one. This mixt. reacted with diisopropyl (tosyloxymethyl)phosphonate in the presence of NaH followed by catalytic hydrogenation and bromotrimethylsilane treatment to afford isomeric 6-amino-3-[2-(phosphonomethoxy)ethyl]purin-2(3H)-one (II) and 2-[2-(phosphonomethoxy)ethoxy]purin-6-amine (III). Similar treatment of compd. I with tritylglycidol gave two isomeric 2-hydroxy-3-(trityloxy)propyl deriv. diisopropyl (tosyloxymethyl)phosphonate to afford protected diester intermediates. These compds. were transformed by hydrogenolysis and ester cleavage with bromotrimethylsilane to the isomeric 6-amino-3-[3-hydroxy-2-(phosphonomethoxy)propyl]-purin-2(3H)-one (IV) and 2-[3-hydroxy-2-(phosphonomethoxy)propoxy]purin-6-amine (V). None of the free phosphonates II-V exhibited any antiviral or cytostatic activity.

L23 ANSWER 26 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213541-78-7 REGISTRY
CN Adenosine 5'-(tetrahydrogen triphosphate), 8-[[13,33,39,59-tetrahydroxy-35-(2-nitrophenyl)-13,33,39,59-tetraoxido-8-oxo-77-[(5'-O-phosphonocytidylyl-(3'.fwdarw.5')-3'-cytidylyl)oxy]-12,14,17,20,23,26,29,32,34,38,40,43,46,49,52,55,58,60,63,66,69,72,75-tricosaoxa-7-aza-13,33,39,59-tetraphosphaheptaheptacont-1-yl]amino]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C83 H146 N14 O65 P10
SR CA
LC STN Files: CA, CAPLUS

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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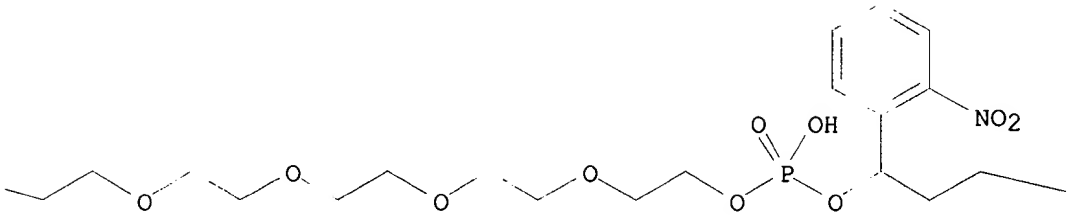

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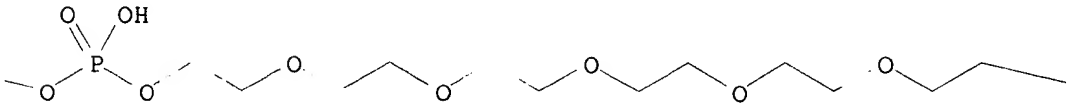
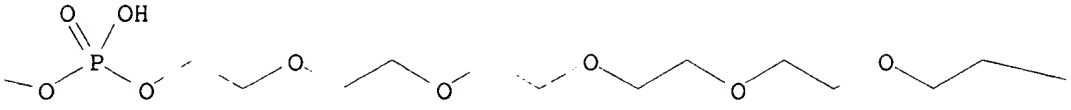


Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-D



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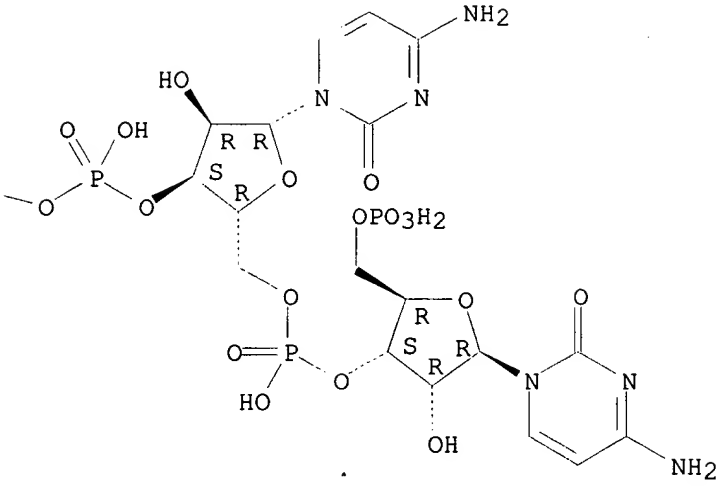


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

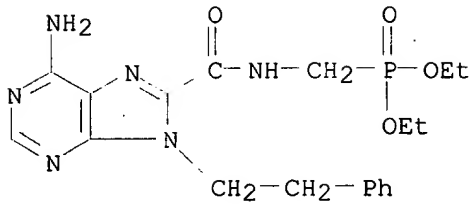
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260732 A novel carboxy-functionalized photo-cleavable dinucleotide analog for the selection of RNA catalysts. Hausch, Felix; Jaschke, Andres (Institut fur Biochemie, Freie Universitat Berlin, Berlin, D-14195, Germany). Tetrahedron Letters, 39(34), 6157-6158 (English) 1998. CODEN: TELEAY. ISSN: 0040-4039. Publisher: Elsevier Science Ltd..

AB A new multifunctional dinucleotide analog is synthesized for the application in in vitro selection expts. with linker-coupled reactants. For this purpose it contains a 5'-pCC ligation site, three flexible hexaethylene glycol spacers, a photo-cleavable o-nitrobenzyl unit and a 3'-terminal carboxy-function which can be derivatized with potential reactants as demonstrated with three model compds.

L23 ANSWER 27 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-43-2 REGISTRY
CN Phosphonic acid, [[[[6-amino-9-(2-phenylethyl)-9H-purin-8-yl]carbonyl]amino]methyl]-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H25 N6 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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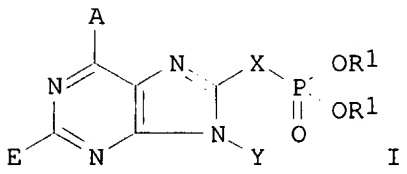

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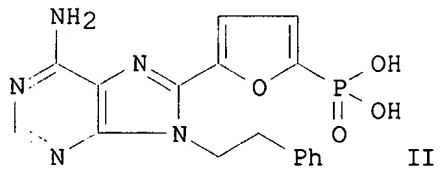


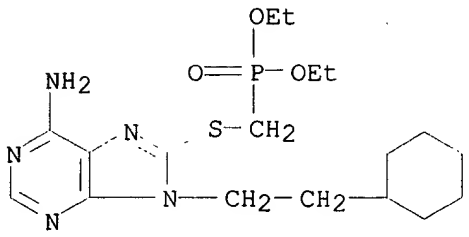
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 28 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-29-4 REGISTRY

Searched by: Mary Hale 308-4258 CM-1 1E01

CN Phosphonic acid, [[[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]thio]methyl]-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H30 N5 O3 P S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

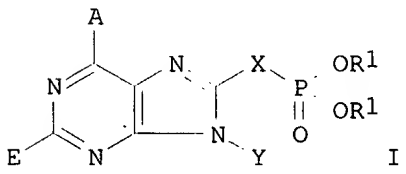


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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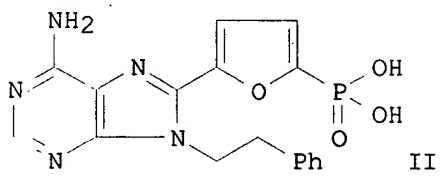

II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus,

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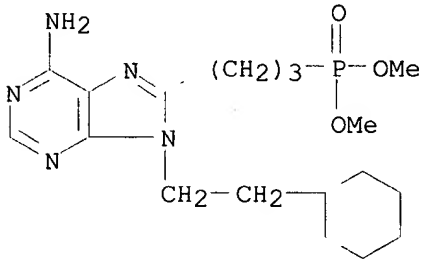
purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 29 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-25-0 REGISTRY
CN Phosphonic acid, [3-[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]propyl]-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H30 N5 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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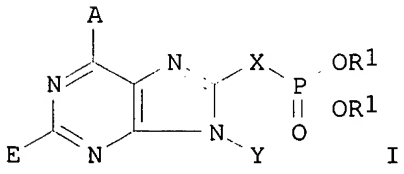

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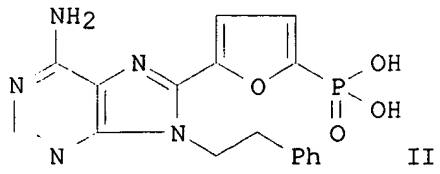


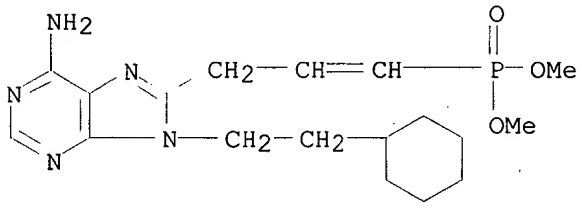
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy),

Searched by: Mary Hale 308-4258 CM-1 1E01

alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 30 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-24-9 REGISTRY
CN Phosphonic acid, [3-[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]-1-propenyl]-, dimethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H28 N5 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

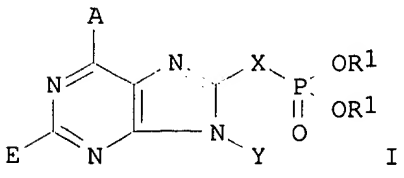


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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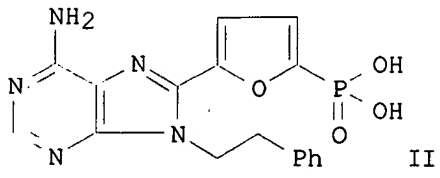
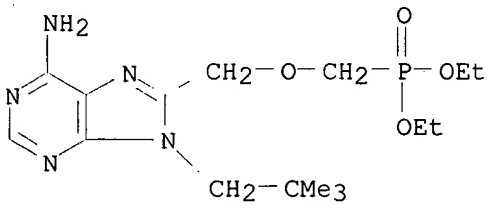


II

Searched by: Mary Hale 308-4258 CM-1 1E01

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 31 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-22-7 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2,2-dimethylpropyl)-9H-purin-8-yl]methoxy]methyl]-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H28 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



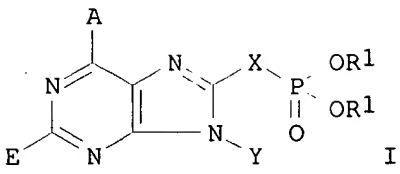
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



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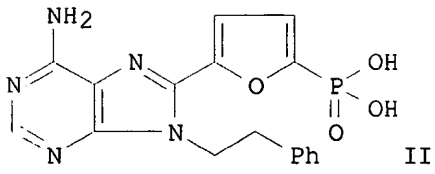
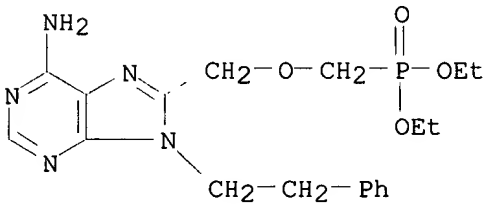


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 32 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-16-9 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2-phenylethyl)-9H-purin-8-yl]methoxy]methyl]-, diethyl ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C19 H26 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

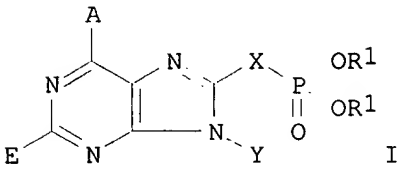
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW:

Searched by: Mary Hale 308-4258 CM-1 1E01

AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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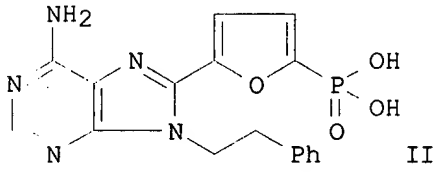
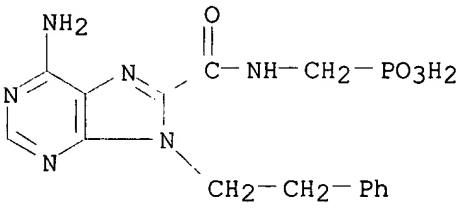


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 33 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213248-07-8 REGISTRY
CN Phosphonic acid, [[[[6-amino-9-(2-phenylethyl)-9H-purin-8-yl]carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H17 N6 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

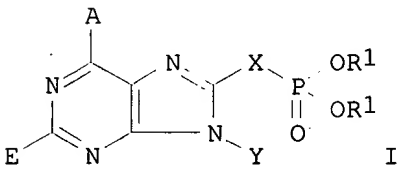
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja

Searched by: Mary Hale 308-4258 CM-1 1E01

(Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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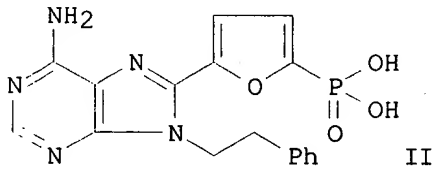
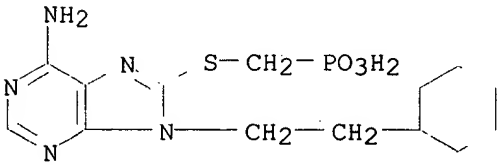


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 34 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-84-8 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]thio]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H22 N5 O3 P S
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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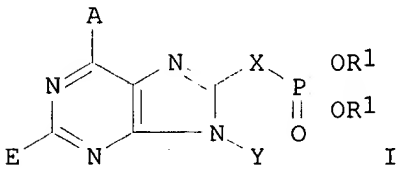

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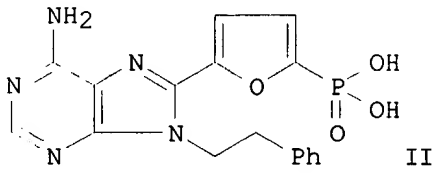
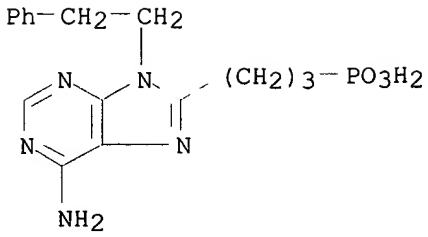


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 35 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-82-6 REGISTRY
CN Phosphonic acid, [3-[6-amino-9-(2-phenylethyl)-9H-purin-8-yl]propyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H20 N5 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 1E01

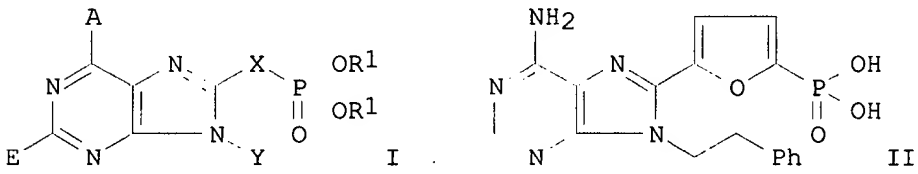


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI

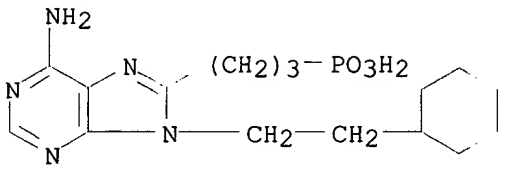


AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 36 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-81-5 REGISTRY

Searched by: Mary Hale 308-4258 CM-1 1E01

CN Phosphonic acid, [3-[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]propyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H26 N5 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

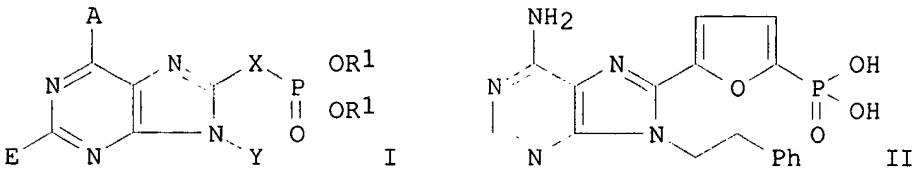


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol.

Searched by: Mary Hale 308-4258 CM-1 1E01

activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 37 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-80-4 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2,2-dimethylpropyl)-9H-purin-8-yl]methoxy]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
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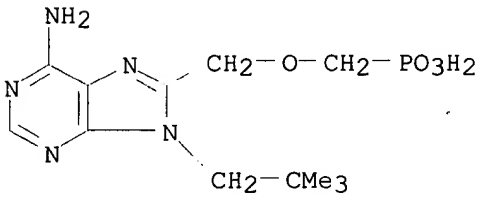
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

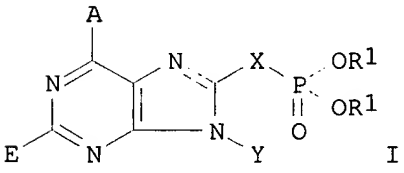


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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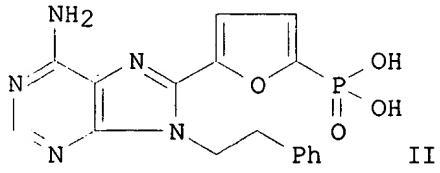


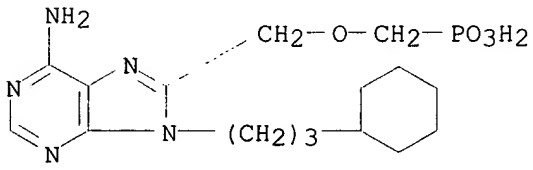
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino,

Searched by: Mary Hale 308-4258 CM-1 1E01

alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 38 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-79-1 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(3-cyclohexylpropyl)-9H-purin-8-yl]methoxy]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H26 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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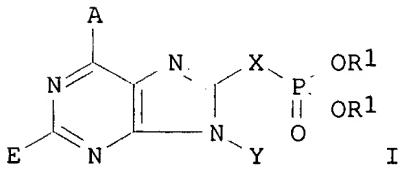

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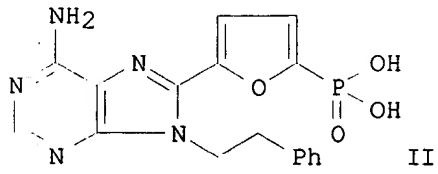


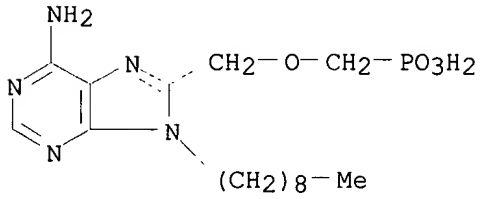
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy),

Searched by: Mary Hale 308-4258 CM-1 1E01

alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 39 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-78-0 REGISTRY
CN Phosphonic acid, [[(6-amino-9-nonyl-9H-purin-8-yl)methoxy]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H28 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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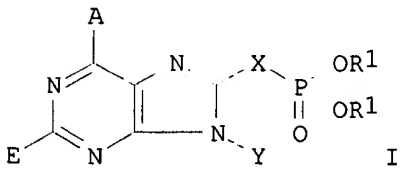

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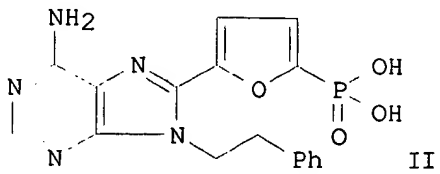
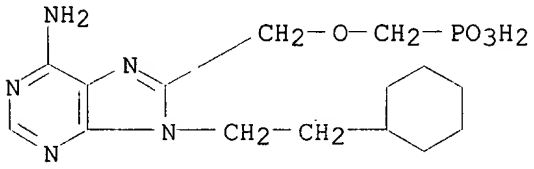


II

Searched by: Mary Hale 308-4258 CM-1 1E01

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 40 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-77-9 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]methoxy]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H24 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

3 REFERENCES IN FILE CA (1967 TO DATE)
3 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 135:348869 Prodrugs phosphorus-containing compounds and pharmacodynamic action. Erion, Mark D.; Reddy, K. Raja; Robinson, Edward D.; Ugarkar, Bheemarao G. (Metabasis Therapeutics, Inc., USA). U.S. US 6312662 B1 20011106, 92 pp., Cont.-in-part of U.S. Ser. No. 263,976. (English). CODEN: USXXAM. APPLICATION: US 1999-392352 19990908. PRIORITY: US 1998-PV77164 19980306; US 1998-PV77165 19980306; US 1999-263976 19990305.

AB The present invention is directed towards novel prodrugs of phosphate, phosphonate, and phosphoramidate compds. which in their active form have a phosphate, phosphonate, or phosphoramidate group, to their prepn., to their synthetic intermediates, and to their uses. More specifically, the invention relates to the area of substituted cyclic 1,3-propanyl phosphate, phosphonate and phosphoramidate esters.

REFERENCE 2: 131:185194 Preparation of cyclic nucleotides as FBPase inhibitor prodrugs. Erion, Mark D.; Reddy, K. Raja; Robinson, Edward D. (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9945016 A2 19990910, 240 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG,

BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, CY, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1999-US4908 19990305. PRIORITY: US 1998-PV77164 19980306; US 1998-PV77165 19980306.

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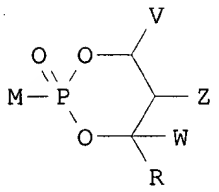

I

AB Prodrugs of phosphorus-contg. nucleotides I, wherein V is selected from the group consisting of H, aralkyl, alicyclic, aryl, substituted aryl, heteroaryl, substituted heteroaryl, 1-alkenyl, 1-alkynyl, and -R9; or together V and Z are connected via 3-5 atoms to form a cyclic group, optionally contg. 1 heteroatom, substituted with hydroxy, acyloxy, alkoxycarbonyloxy, or aryloxycarbonyloxy attached to a carbon atom that is three atoms from an oxygen attached to the phosphorus; or together V and Z are connected via 3-5 atoms to form a cyclic group, optionally contg. 1 heteroatom, that is fused to an aryl group at the beta and gamma position to the oxygen attached to the phosphorus. Together V and W are connected via 3 carbon atoms to form an optionally substituted cyclic group contg. 6 carbon atoms and substituted with one substituent selected from the group consisting of hydroxy, acyloxy, alkoxycarbonyloxy, alkylthiocarbonyloxy, and aryloxycarbonyloxy, attached to a carbon atom that is three atoms from an oxygen attached to the phosphorus; W and R are independently selected from the group consisting of H, alkyl, aralkyl, alicyclic, aryl, substituted aryl, heteroaryl, substituted heteroaryl, 1-alkenyl, 1-alkynyl, and -R9. Z is selected from the group consisting of -CHR2OH, -CHR2OC(O)R3, -CHR2OC(S)R3, -CHR2OC(S)OR3, -CHR2OC(O)SR3, -CHR2OCO2R3, -OR2, -SR2, -CHR2N3, -CH2aryl, -CH(aryl)OH, -CH(CH=CR22)OH, -CH(C.tplbond.CR2)OH, -R2, -NR22, -OCOR3, -OCO2R3, -SCOR3, -SCO2R3, -NHCOR2, -NHCO2R3, -CH2NHaryl, (CH2)p-OR2, and (CH2)p-SR2; -R2 is an R3 or -H; R3 is selected from the group consisting of alkyl, aryl, aralkyl, and alicyclic; and R9 is selected from the group consisting of alkyl, aralkyl, and alicyclic; p is an integer from 2 to 3. With the proviso that (a) V, Z, W, and R are not all -H; and (b) when Z is -R2, then at least one of V and W is not -H, or -R9; and M is selected from the group that attached to PO32-, P2O63-, or P3O94- is biol. active in vivo, and that is attached to the phosphorus in I via a carbon, oxygen, or nitrogen atom; and pharmaceutically acceptable prodrugs and salts thereof. Thus, cyclic nucleotide I (M = adenine-9-.beta.-D-arabinofuranos-5'-yl; V = 4-pyridyl; Z = W = R = H) was prepd. and tested as prodrug human liver FBPase inhibitor (EC50 < 10 .mu.M).

REFERENCE 3: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG,

BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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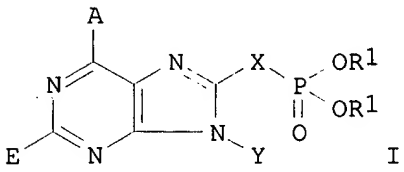

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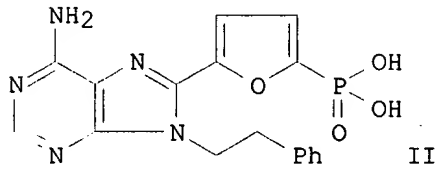
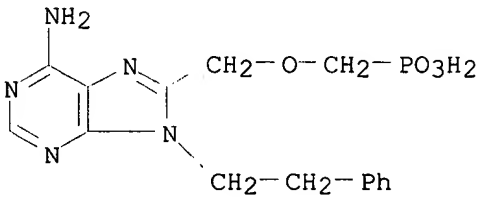


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 41 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-75-7 REGISTRY
CN Phosphonic acid, [[[6-amino-9-(2-phenylethyl)-9H-purin-8-yl]methoxy]methyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H18 N5 O4 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

Searched by: Mary Hale 308-4258 CM-1 1E01

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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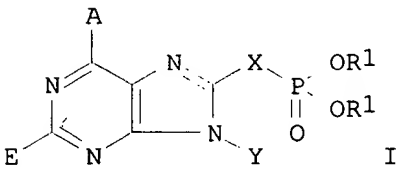

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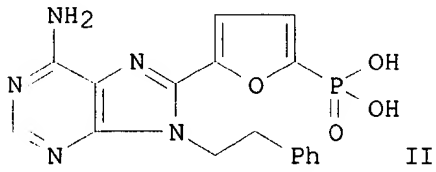


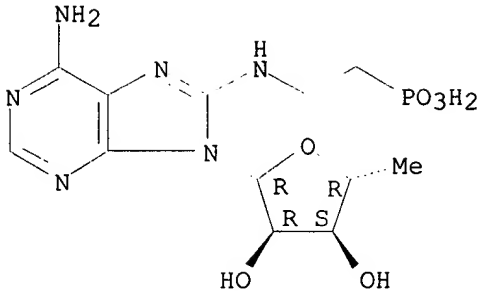
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 42 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-73-5 REGISTRY
CN Phosphonic acid, [2-[[6-amino-9-(5-deoxy-.beta.-D-ribofuranosyl)-9H-purin-8-yl]amino]ethyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H19 N6 O6 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

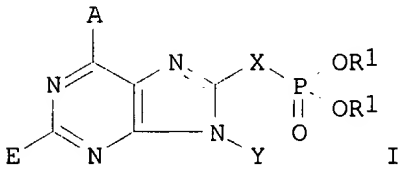


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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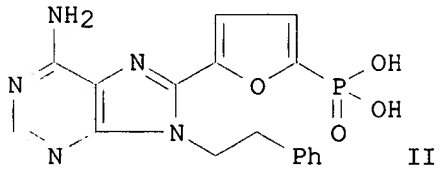


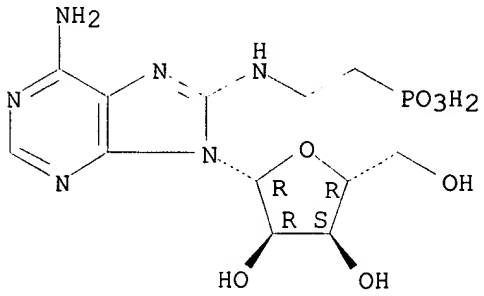
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

Searched by: Mary Hale 308-4258 CM-1 1E01

L23 ANSWER 43 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-71-3 REGISTRY
CN Phosphonic acid, [2-[(6-amino-9-.beta.-D-ribofuranosyl-9H-purin-8-yl)amino]ethyl]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C12 H19 N6 O7 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

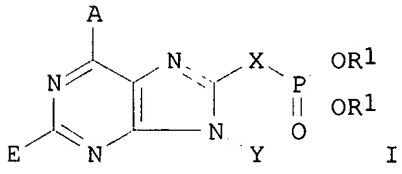


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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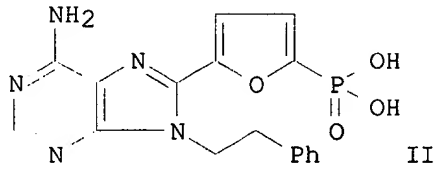


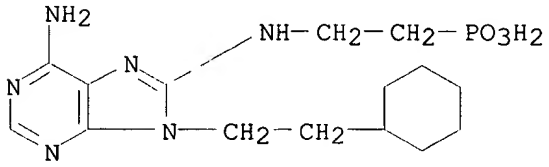
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl,

Searched by: Mary Hale 308-4258 CM-1 1E01

aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 44 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-69-9 REGISTRY
CN Phosphonic acid, [2-[[6-amino-9-(2-cyclohexylethyl)-9H-purin-8-yl]amino]ethyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H25 N6 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

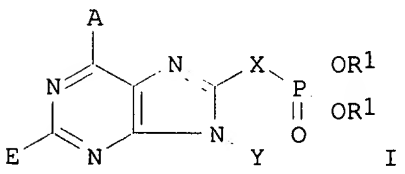


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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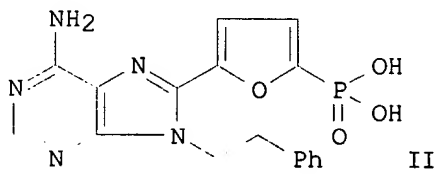


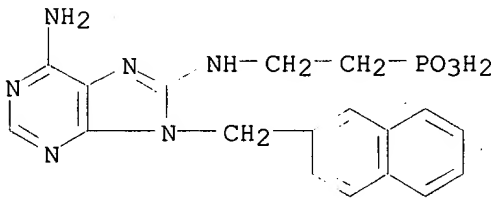
II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl,

Searched by: Mary Hale 308-4258 CM-1 1E01

carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 45 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-67-7 REGISTRY
CN Phosphonic acid, [2-[[6-amino-9-(2-naphthalenylmethyl)-9H-purin-8-yl]amino]ethyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C18 H19 N6 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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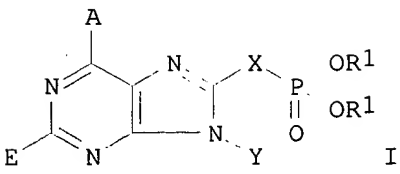
Searched by: Mary Hale 308-4258 CM-1 1E01



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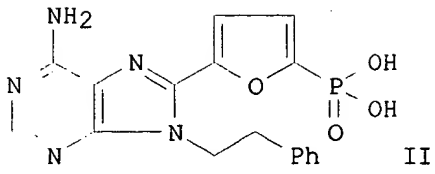
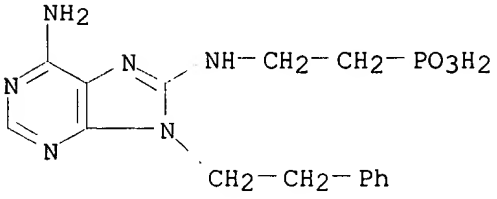


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 46 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-66-6 REGISTRY
CN Phosphonic acid, [2-[[6-amino-9-(2-phenylethyl)-9H-purin-8-yl]amino]ethyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C15 H19 N6 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja (Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW:

Searched by: Mary Hale 308-4258 CM-1 1E01

AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

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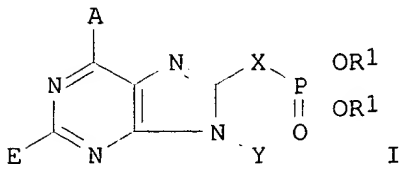

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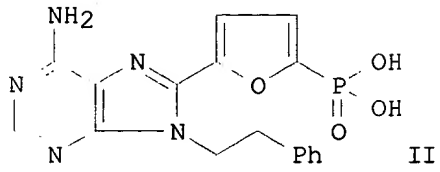
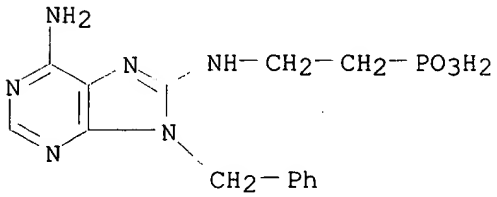


II

AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 47 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 213247-64-4 REGISTRY
CN Phosphonic acid, [2-[[6-amino-9-(phenylmethyl)-9H-purin-8-yl]amino]ethyl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C14 H17 N6 O3 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

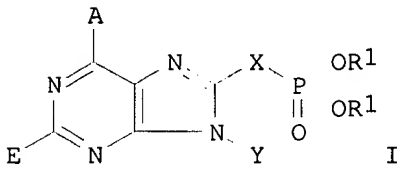
1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 129:260281 Preparation of novel purines for use as inhibitors of fructose-1,6-bisphosphatase. Dang, Qun; Erion, Mark D.; Reddy, M. Rami; Robinsion, Edward D.; Kasibhatla, Srinivas Rao; Reddy, K. Raja

Searched by: Mary Hale 308-4258 CM-1 1E01

(Metabasis Therapeutics, Inc., USA). PCT Int. Appl. WO 9839344 A1 19980911, 126 pp. DESIGNATED STATES: W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM; RW: AT, BE, BF, BJ, CF, CG, CH, CI, CM, DE, DK, ES, FI, FR, GA, GB, GR, IE, IT, LU, MC, ML, MR, NE, NL, PT, SE, SN, TD, TG. (English). CODEN: PIXXD2. APPLICATION: WO 1998-US4502 19980306. PRIORITY: US 1997-40623 19970307.

GI



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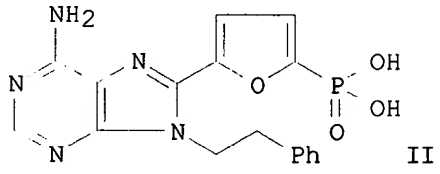


II

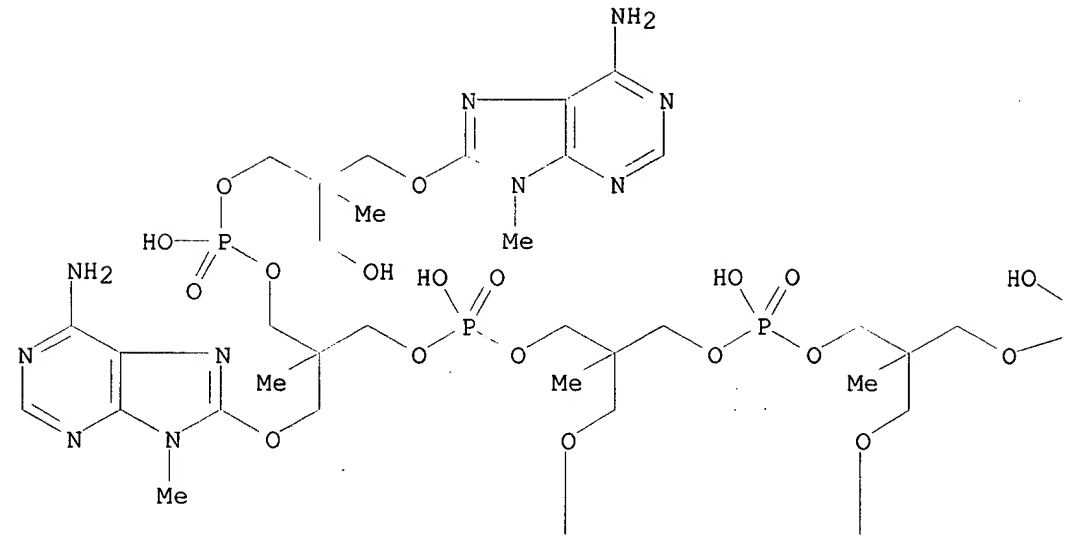
AB Purines I [A = H, amino, sulfonylamino, alkoxy, alkylthio, halogen, alkyl, carbamoyl, guanidine, amidine, perhaloalkyl; E = H, halogen, alkylthio, perhaloalkyl, alkyl, alkenyl, alkynyl, alkoxy, CN, amino; X = alkylamino, alkyl, alkenyl, alkynyl, alkyl(carboxyl), alkyl(hydroxy), alkyl(phosphonate), alkyl(sulfonate), aryl, alkylaminoalkyl, alkoxyalkyl, alkylthioalkyl, alkylthio, alicyclic, 1,1-dihaloalkyl, carbonylalkyl, aminocarbonylamino, alkylaminocarbonyl, alkylcarbonylamino, aralkyl, and alkylaryl; Y = H, alkyl, alkenyl, alkynyl, aryl, alicyclic, aralkyl, aryloxyalkyl, alkoxyalkyl, acyl, sulfonyl, carboxyl, carbamoyl, amino, alkoxy; XY = cyclic group including cyclic alkyl, heterocyclic, and aryl; R1 = H, alkyl, aryl, alicyclic; R1R1 = cyclic group including cyclic alkyl, heterocyclic] were prepd. for use as fructose-1,6-bisphosphatase (FBPase) inhibitors for treatment of carbohydrate metab. disorders. Thus, purine II starting from 5-amino-4,6-dichloropyrimidine, phenethylamine, and 2-furaldehyde. The prepd. compds. were tested for a variety of biol. activities including inhibition of FBPase and activity toward AMP binding enzymes such as adenosine kinase.

L23 ANSWER 48 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 164992-27-2 REGISTRY
CN 5'-Adenylic acid, 2'-deoxy-, mono[2,8,14,20,26,32,38,44,50-nonakis[[(6-amino-9-methyl-9H-purin-8-yl)oxy]methyl]-5,11,17,23,29,35,41,47,51-nonahydroxy-2,8,14,20,26,32,38,44,50-nonamethyl-5,11,17,23,29,35,41,47-octaoxido-4,6,10,12,16,18,22,24,28,30,34,36,40,42,46,48-hexadecaoxa-5,11,17,23,29,35,41,47-octaphosphahenpentacont-1-yl] ester (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN 5'-Adenylic acid, 2'-deoxy-, mono[2,8,14,20,26,32,38,44,50-nonakis[[(6-amino-9-methyl-9H-purin-8-yl)oxy]methyl]-5,11,17,23,29,35,41,47,51-nonahydroxy-2,8,14,20,26,32,38,44,50-nonamethyl-4,6,10,12,16,18,22,24,28,30,34,36,40,42,46,48-hexadecaoxa-5,11,17,23,29,35,41,47-octaphosphahenpentacont-1-yl] ester, P',P'',P''',P'''',P''''',P'''''',P''''''',P'''''''-octaoxide
FS STEREOSEARCH
MF C109 H157 N50 O48 P9
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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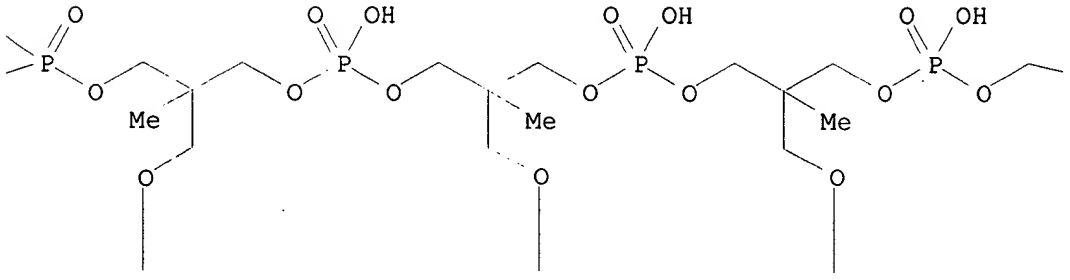
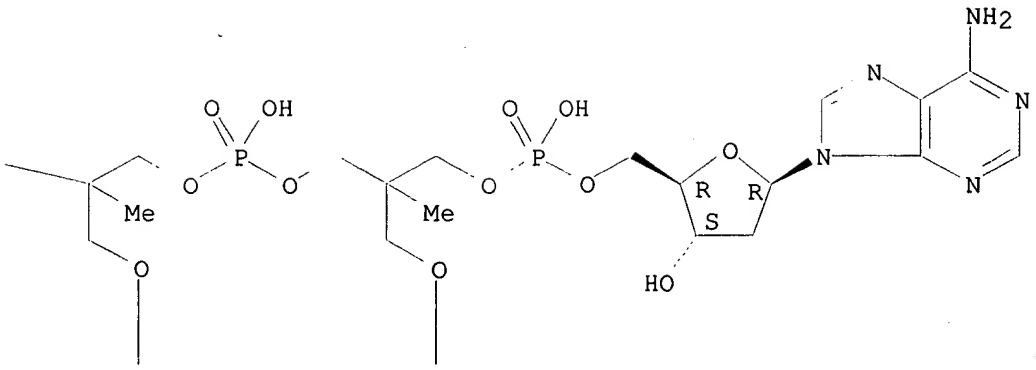
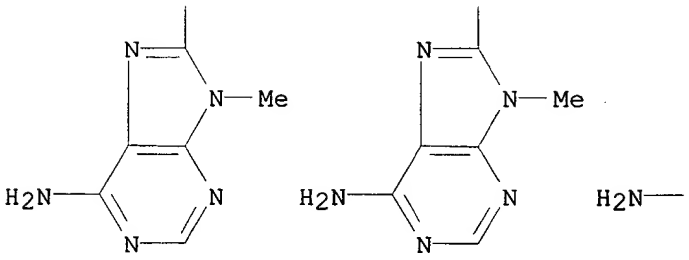


Searched by: Mary Hale 308-4258 CM-1 1E01

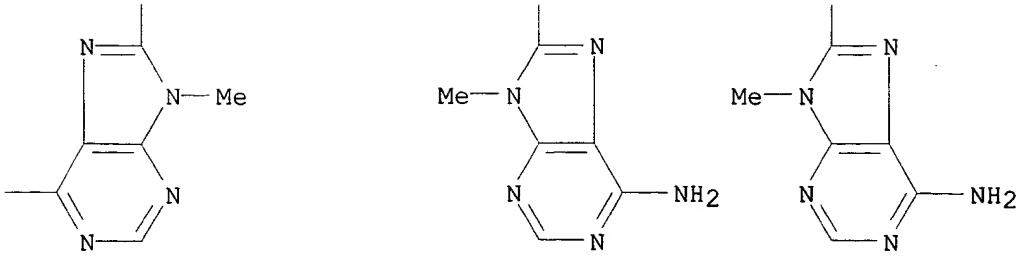
PAGE 1-C



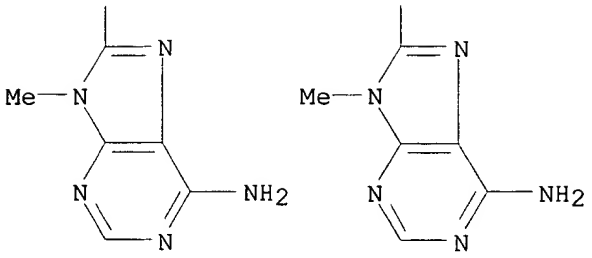
PAGE 2-A



PAGE 2-B



Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:83946 Preparation of acyclic nucleoside analogs and antisense oligonucleotide sequences containing them. Cook, Philip D.; Delecki, Daniel J.; Guinosso, Charles (Sterling Winthrop Inc., USA). PCT Int. Appl. WO 9422864 A1 19941013, 37 pp. DESIGNATED STATES: W: AU, BR, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK, UA; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1994-US2995 19940321. PRIORITY: US 1993-40326 19930330.

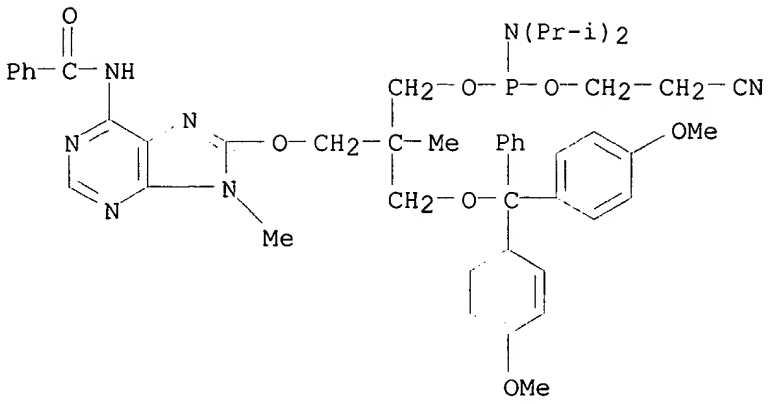
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Acyclic nucleoside analogs (I; R1 = H or a blocking group that is compatible with oligonucleotide synthesis; R2 = H, Me; R3 = H, P(R4)OR5; wherein R4 = Cl, 4-nitroimidazole, imidazole, tetrazole, triazole, or di(lower-alkyl)amino; R5 = Me, 2-cyanoethyl, or 2,2,2-trichloroethyl; n = 0 - 2; X = O, S, or NR6; wherein R6 = H, lower alkyl; Q is chosen from the group consisting of Q1 and Q2; wherein R7 = lower alkyl; R8 = H, benzoyl, anisoyl, or lower alkylcarbonyl) and its pharmaceutically acceptable addn. salts are prepd. Modified oligonucleotides contg. the nucleoside analogs of formula I are stable to nuclease degrdn. and are useful in inhibiting gene expression, in sequencing, and in mutagenesis. Thus, an oligomer 5'-CCTTCTCA*GTCGGA*C-3' (II; A* = acyclic nucleoside residue Q2) was synthesized by using std. procedures on a DNA synthesizer (Applied Biosystems model 380B) and an acyclic nucleoside phosphoramidite (III; DMT = dimethoxytrityl) (prepn. given). Using rabbit reticulocyte lysate, II at 30 .mu.M inhibited cell free-translation of rabbit .alpha.-globin mRNA by 74.+-.10% in the absence of RNase H and 84.+-.5% in the presence of RNase H.

L23 ANSWER 49 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 163707-01-5 REGISTRY
CN Phosphoramidous acid, bis(1-methylethyl)-, 3-[[6-(benzoylamino)-9-methyl-9H-purin-8-yl]oxy]-2-[[bis(4-methoxyphenyl)phenylmethoxy]methyl]-2-methylpropyl 2-cyanoethyl ester (9CI) (CA INDEX NAME)
MF C48 H56 N7 O7 P
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER, USPATFULL

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 123:83946 Preparation of acyclic nucleoside analogs and antisense oligonucleotide sequences containing them. Cook, Philip D.; Delecki, Daniel J.; Guinosso, Charles (Sterling Winthrop Inc., USA). PCT Int. Appl. WO 9422864 A1 19941013, 37 pp. DESIGNATED STATES: W: AU, BR, CA, CZ, FI, HU, JP, KR, NO, NZ, RU, SK, UA; RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE. (English). CODEN: PIXXD2. APPLICATION: WO 1994-US2995 19940321. PRIORITY: US 1993-40326 19930330.

GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Acyclic nucleoside analogs (I; R1 = H or a blocking group that is compatible with oligonucleotide synthesis; R2 = H, Me; R3 = H, P(R4)OR5; wherein R4 = Cl, 4-nitroimidazole, imidazole, tetrazole, triazole, or di(lower-alkyl)amino; R5 = Me, 2-cyanoethyl, or 2,2,2-trichloroethyl; n = 0 - 2; X = O, S, or NR6; wherein R6 = H, lower alkyl; Q is chosen from the group consisting of Q1 and Q2; wherein R7 = lower alkyl; R8 = H, benzoyl, anisoyl, or lower alkylcarbonyl) and its pharmaceutically acceptable addn. salts are prepd. Modified oligonucleotides contg. the nucleoside analogs of formula I are stable to nuclease degrdn. and are useful in inhibiting gene expression, in sequencing, and in mutagenesis. Thus, an oligomer 5'-CCTTCTCA*GTCGGA*C-3' (II; A* = acyclic nucleoside residue Q2) was synthesized by using std. procedures on a DNA synthesizer (Applied Biosystems model 380B) and an acyclic nucleoside phosphoramidite (III; DMT = dimethoxytrityl) (prepn. given). Using rabbit reticulocyte lysate, II at 30 .mu.M inhibited cell free-translation of rabbit .alpha.-globin mRNA by 74.+-.10% in the absence of RNase H and 84.+-.5% in the presence of RNase H.

L23 ANSWER 50 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 128191-38-8 REGISTRY
CN Uridine, N-benzoyl-3'-O-[(1,1-dimethylethyl)dimethylsilyl]-5'-O-[(4-methoxyphenyl)diphenylmethyl]-P-methyladenylyl-(2'.fwdarw.5')-, 2',3'-diacetate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Adenosine, 2',3'-di-O-acetyl-P-methyluridylyl-(5'.fwdarw.2')-N-benzoyl-3'-

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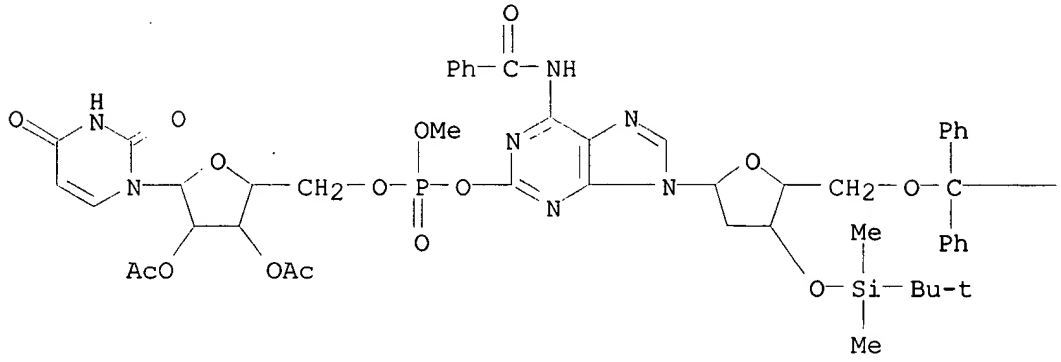
O-[(1,1-dimethylethyl)dimethylsilyl]-5'-O-[(4-
methoxyphenyl)diphenylmethyl]-
MF C57 H64 N7 O16 P Si
SR CA
LC STN Files: CA, CAPLUS

PAGE 1-A



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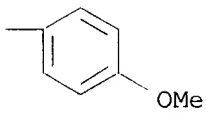
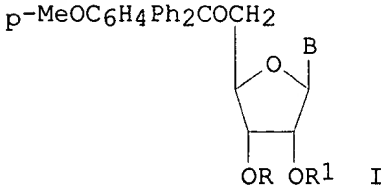


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 113:97966 A study on the alkylsilyl groups in oligoribonucleotide synthesis. Wu, Taifeng; Ogilvie, Kelvin K. (Dep. Chem., McGill Univ., Montreal, PQ, H3A 2K6, Can.). J. Org. Chem., 55(15), 4717-24 (English) 1990. CODEN: JOCEAH. ISSN: 0022-3263.

GI



I

AB A detailed study was carried out to show that the fidelity of the 3'-5' phosphate linkage is preserved during oligoribonucleotide synthesis when

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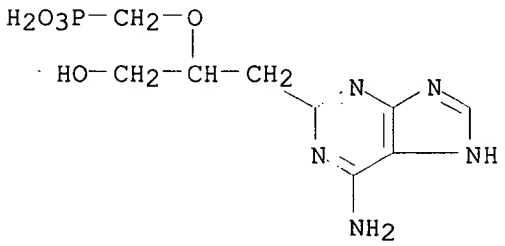
alkylsilyl groups are used to protect the 2'-hydroxyl groups. The isomeric purity of the 2'-silylated ribonucleoside 3'-phosphoramidites [I; B = N 6-benzoyladenine, R = P(OMe)N(CHMe2)2, R1 = SiMe2(Me3; B = N4-benzoylcytosine, R = P(OMe)N(CHMe2)2, R1 = SiMe2(CMe3); B = N2-phenoxyacetylguanine, R = P(OMe)N(CHMe2)2, R1 = Si(CHMe2)3; B = uracil, R = P(OMe)N(CHMe2)2, R1 = SiMe2CMe3] the key intermediates in oligoribonucleotide synthesis, were established by comparing them with the 3'-silylated ribonucleoside 2'-phosphoramidites [I; B = N6-benzoyladenine, R = SiMe2CMe3; R1 = P(OMe)N(CHMe2)2; B = N4-benzoylcytosine, R = SiMe2CMe3, R1 = SiMe2CMe3, R1 = P(OMe)N(CHMe2)2; B = N2-phenoxyacetylguanine, R = Si(CHMe2)3, R1 = P(OMe)N(CHMe2)2; B = uracil, R = SiMe2(Me3), R1 = P(OMe)N(CHMe)2] using 1H- and 31P-NMR spectroscopy. Using these 3'-amidites, a series of natural dinucleotides (ApU, CpU, GpU, UpU) were synthesized in soln. Isomeric dinucleotides with 2'-5' phosphate linkages (ApU, CpU, GpU, UpU) were prepd. using the 3'-silylated nucleoside 2'-phosphoramidites. The intermediates using the syntheses and the final products were characterized by 1H- and 31P-NMR spectroscopy and HPLC. Comparison of the data from these two series of compds. provided unambiguous evidence for the fidelity of phosphate linkages in both the intermediates and the final products. To complete the comparison, a dinucleotide (UpU) was prepd. on a solid support.

L23 ANSWER 51 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 118552-99-1 REGISTRY
CN Phosphonic acid, [[2-(6-amino-1H-purin-2-yl)-1-(hydroxymethyl)ethoxy]methyl]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phosphonic acid, [[2-(6-amino-1H-purin-2-yl)-1-(hydroxymethyl)ethoxy]methyl]-, (.+-.)-
FS 3D CONCORD
MF C9 H14 N5 O5 P
SR CA
LC STN Files: CA, CAPLUS, USPATFULL



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 110:75170 Preparation and testing of N-phosphonylmethoxyalkyl derivatives of pyrimidine and purine bases with antiviral activity. Holy, Antonin; Rosenberg, Ivan; De Clercq, Erik (Ceskoslovenska Akademie Ved, Czech.; Rega Foundation). Eur. Pat. Appl. EP 253412 A2 19880120, 15 pp. DESIGNATED STATES: R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE. (English). CODEN: EPXXDW. APPLICATION: EP 1987-110399 19870717. PRIORITY: CS 1986-5469 19860718.
AB BCH2CHROCH2P(:O)(OH)2 (I) [R = H, CH2OH; B = (substituted) pyrimidin-1-yl, pyrimidin-3-yl, purin-3-yl, purin-7-yl, purin-9-yl, excluding adenin-9-yl], useful as virucides, were prepd. Isoamyl nitrite was added

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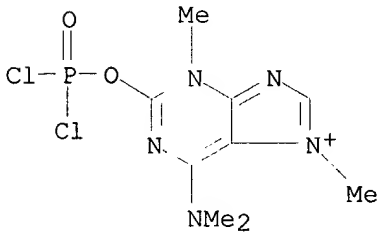
to 9-(2-phosphonylmethoxyethyl)adenine in HOAc and the mixt. was allowed to stand 72 h at room temp. to give 9-(2-phosphonylmethoxyethyl)hypoxanthine. I had IC50's of 7-150 .mu.g/mL against HSV-1, vs 0.02 .mu.g/mL for 5-(2-bromovinyl)-2'-deoxyuridine.

L23 ANSWER 52 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 54901-41-6 REGISTRY
CN 3H-Purinium, 2-[(dichlorophosphinyl)oxy]-6-(dimethylamino)-3,7-dimethyl-, phosphorodichloridate (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phosphorodichloridate, 2-[(dichlorophosphinyl)oxy]-6-(dimethylamino)-3,7-dimethyl-3H-purinium (9CI)
MF C9 H13 Cl2 N5 O2 P . Cl2 O2 P
LC STN Files: CA, CAPLUS

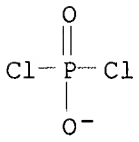
CM 1

CRN 54901-40-5
CMF C9 H13 Cl2 N5 O2 P



CM 2

CRN 47986-81-2
CMF Cl2 O2 P

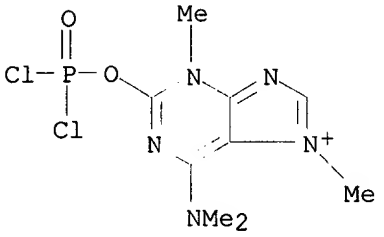


1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

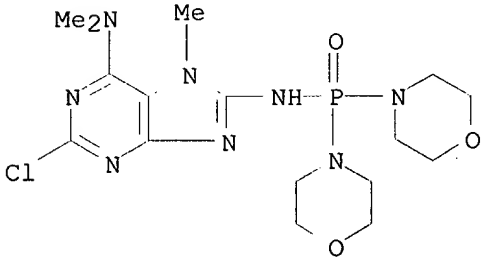
REFERENCE 1: 82:72938 Syntheses in purine derivatives. XXXIX. New synthesis of C-iminopurines. Kozlova, O. V.; Nikolaeva, L. A.; Ovcharova, I. M.; Persiyanova, I. V.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 8(10), 32-6 (Russian) 1974. CODEN: KHFZAN.
GI For diagram(s), see printed CA Issue.
AB The dihydropurinium chloride I (R = R1 = MeNH; X = Cl) was prepd. by treating either 2-ethoxy-3,7-dimethylhypoxanthine or 6-ethoxy-2-oxo-2,3-dihydro-3,7-dimethylpurine with POCl3 and then with MeNH2: I (R = MeNH, R1 = EtO; R1 = MeNH, R = MeO, EtO, PrO; X = Cl) were prepd. by treating I [R = MeNH, R1 = Cl2P(O)O; R1 = MeNH, R = Cl2P(O)O; X = Cl2P(O)O] with the appropriate Na alcoholate. Sequential treatment of either 2-(dimethylamino)-3,7-dimethylhypoxanthine or 6-(dimethylamino)-2-oxo-2,3-dihydro-3,7-dimethylpurine with POCl3 and Me2NH gave I (R = R1 = Me2N; X =

Cl).

L23 ANSWER 53 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 54901-40-5 REGISTRY
CN 3H-Purinium, 2-[(dichlorophosphinyl)oxy]-6-(dimethylamino)-3,7-dimethyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C9 H13 Cl2 N5 O2 P
CI COM



L23 ANSWER 54 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 38137-07-4 REGISTRY
CN Phosphinic amide, N-[2-chloro-6-(dimethylamino)-7-methyl-7H-purin-8-yl]-P,P-di-4-morpholinyl- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C16 H26 Cl N8 O3 P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:88447 Syntheses of purines. XXIX. 8- and 2-[bis(aziridino)phosphinamido]purines. Korsunskii, V. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(6), 28-31 (Russian) 1972. CODEN: KHFZAN.
GI For diagram(s), see printed CA Issue.
AB 2,6-Dichloro-8-amino-7-methylpurine (I, R = R1 = Cl, R2 = NH2) (II) was converted to the corresponding I (R = Me2N, morpholino, piperidino) by heating with excess amine; these gave the resp. I [R2 = bis(aziridino)phosphinamido, dimorpholinophosphinamido] with POCl3 and then amine-Et3N in C6H6. Redn. of I (R = morpholino, piperidino; R1 = Cl; R2 = NH2) with red P and HI afforded the corresponding I (R1 = H), which yielded the I [R2 = bis(aziridino)phosphinamido] as above. I [R = R1 = H, R2 = bis(aziridino)phosphinamido] was prepd. analogously from I (R = R1 =

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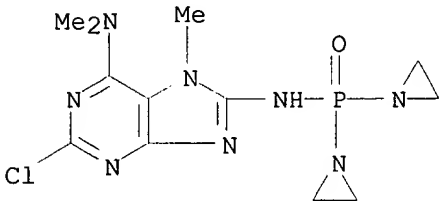
H, R2 = NH2). Re-fluxing II with 40% aq. NaOH gave I (R = OH, R1 = Cl, R2 = NH2), which reacted with POCl3 and then aq. NH3 to give I (R = Cl, R1 = NH2, R2 = H); the latter gave I (R = Me2N, R1 = NH2, R2 = H) (III) with aq. Me2NH. I [R = Me2N, R1 = bis(aziridino)phosphinamido, R2 = H] was formed as above from III.

L23 ANSWER 55 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 38137-06-3 REGISTRY
CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-[2-chloro-6-(dimethylamino)-7-methyl-7H-purin-8-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H18 Cl N8 O P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)



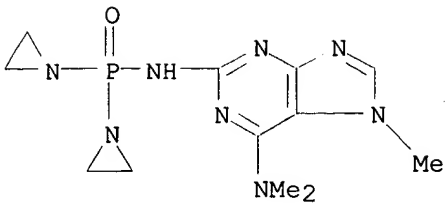
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:88447 Syntheses of purines. XXIX. 8- and 2-[bis(aziridino)phosphinamido]purines. Korsunskii, V. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(6), 28-31 (Russian) 1972. CODEN: KHFZAN.
GI For diagram(s), see printed CA Issue.
AB 2,6-Dichloro-8-amino-7-methylpurine (I, R = R1 = Cl, R2 = NH2) (II) was converted to the corresponding I (R = Me2N, morpholino, piperidino) by heating with excess amine; these gave the resp. I [R2 = bis(aziridino)phosphinamido, dimorpholinophosphinamido] with POCl3 and then amine-Et3N in C6H6. Redn. of I (R = morpholino, piperidino; R1 = Cl; R2 = NH2) with red P and HI afforded the corresponding I (R1 = H), which yielded the I [R2 = bis(aziridino)phosphinamido] as above. I [R = R1 = H, R2 = bis(aziridino)phosphinamido] was prepd. analogously from I (R = R1 = H, R2 = NH2). Re-fluxing II with 40% aq. NaOH gave I (R = OH, R1 = Cl, R2 = NH2), which reacted with POCl3 and then aq. NH3 to give I (R = Cl, R1 = NH2, R2 = H); the latter gave I (R = Me2N, R1 = NH2, R2 = H) (III) with aq. Me2NH. I [R = Me2N, R1 = bis(aziridino)phosphinamido, R2 = H] was formed as above from III.

L23 ANSWER 56 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 38119-35-6 REGISTRY
CN Phosphinic amide, P,P-bis(1-aziridinyl)-N-[6-(dimethylamino)-7-methyl-7H-purin-2-yl]- (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C12 H19 N8 O P
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Searched by: Mary Hale 308-4258 CM-1 1E01

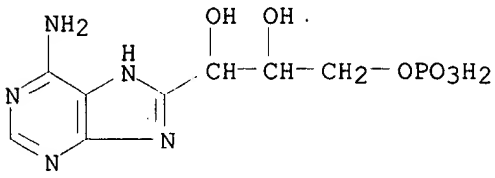


PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 77:88447 Syntheses of purines. XXIX. 8- and 2-[bis(aziridino)phosphinamido]purines. Korsunskii, V. S.; Golovchinskaya, E. S. (Vses. Nauchno-Issled. Khim.-Farm. Inst. im. Ordzhonikidze, Moscow, USSR). Khim.-Farm. Zh., 6(6), 28-31 (Russian) 1972. CODEN: KHFZAN.
GI For diagram(s), see printed CA Issue.
AB 2,6-Dichloro-8-amino-7-methylpurine (I, R = R1 = Cl, R2 = NH2) (II) was converted to the corresponding I (R = Me2N, morpholino, piperidino) by heating with excess amine; these gave the resp. I [R2 = bis(aziridino)phosphinamido, dimorpholinophosphinamido] with POCl3 and then amine-Et3N in C6H6. Redn. of I (R = morpholino, piperidino; R1 = Cl; R2 = NH2) with red P and HI afforded the corresponding I (R1 = H), which yielded the I [R2 = bis(aziridino)phosphinamido] as above. I [R = R1 = H, R2 = bis(aziridino)phosphinamido] was prepd. analogously from I (R = R1 = H, R2 = NH2). Re-fluxing II with 40% aq. NaOH gave I (R = OH, R1 = Cl, R2 = NH2), which reacted with POCl3 and then aq. NH3 to give I (R = Cl, R1 = NH2, R2 = H); the latter gave I (R = Me2N, R1 = NH2, R2 = H) (III) with aq. Me2NH. I [R = Me2N, R1 = bis(aziridino)phosphinamido, R2 = H] was formed as above from III.

L23 ANSWER 57 OF 57 REGISTRY COPYRIGHT 2002 ACS
RN 28786-14-3 REGISTRY
CN 1,2,3-Propanetriol, 1-(6-aminopurin-8-yl)-, 3-(dihydrogen phosphate) (8CI) (CA INDEX NAME)
OTHER NAMES:
CN 1-(8-Adenyl) 3-glycerophosphate
FS 3D CONCORD
MF C8 H12 N5 O6 P
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 73:20400 Intramolecular dimerization reaction in x-ray irradiation of purine nucleotides. Keck, Klaus (Inst. Strahlenchem.,

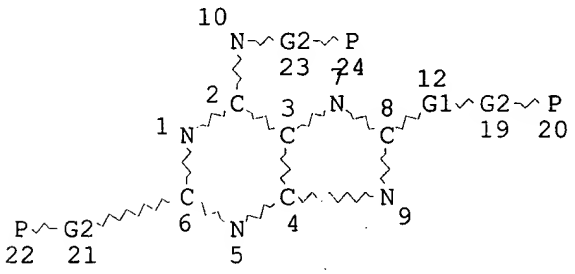
Searched by: Mary Hale 308-4258 CM-1 1E01

Kernforschungszentrum Karlsruhe, Karlsruhe, Ger.). Mol. Strukt. Strahlenwirkung, Jahrestag. Deut. Ges. Biophys., Tagungsber., Meeting Date 1966, 84-7. Editor(s): Glubrecht, H. Georg Thieme Verlag: Stuttgart, Ger. (German) 1968. CODEN: 17RYAN.

AB A reaction is reported in which the accepted reaction scheme for radiolysis of nucleotides in H2O soln. does not take place. A 5 .times. 10-3 M H2O soln. of AMP was irradiated under N with x-rays or .gamma.-rays in the dose range 1-4 megarads. The resulting soln. was chromatographed on an ion exchange column and and the uv absorption recorded at 254 nm. Five fractions were sepd., 4 of which were easily identifiable. The 5th fraction, unknown, was subjected to structural analyses; its uv spectrum, at all pH values, is very similar to that of AMP and is displaced only approx. 5 nm in the long wavelength region. Analyses show that all 3 components of the unknown nucleotide-base, sugar, and phosphate groups are intact. Therefore, it is assumed that through the irradn., a new bond is formed between the adenine and ribose parts. The linkage site on the base is C8, proven through NMR spectra in which a signal is absent for protons on C8 of the adenine residue. The position of the new bond on the ribose is C3. The compd. is identified as 1-(8-adenyl) 3-glycerophosphate. The compd. is formed under acid conditions from 1-(8-adenyl) 1-glycerophosphate through migration of the phosphate group.

=> d l30 que stat;d l31 que stat;d l32 que stat

L24 STR



VAR G1=X/O/S/N/C
REP G2=(0-20) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

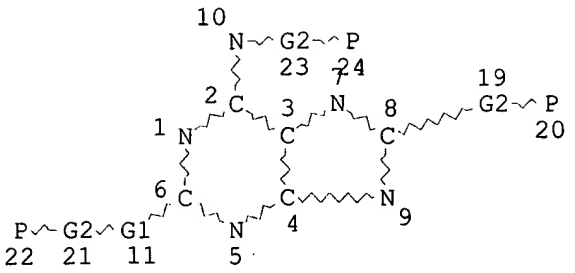
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L30 0 SEA FILE=REGISTRY SSS FUL L24

100.0% PROCESSED 34049 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.02

L25 STR

Searched by: Mary Hale 308-4258 CM-1 1E01



VAR G1=X/O/S/N/C
REP G2=(0-20) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 17

STEREO ATTRIBUTES: NONE
L31 0 SEA FILE=REGISTRY SSS FUL L25

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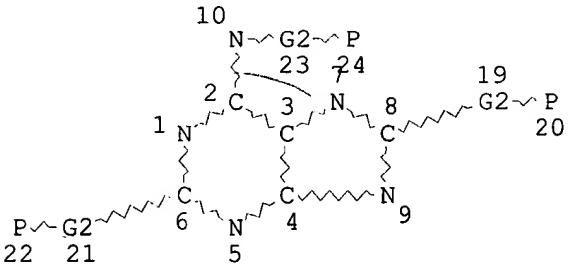
SEARCH TIME: 00.00.02

L26 STR



REP G2=(0-20) A
NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

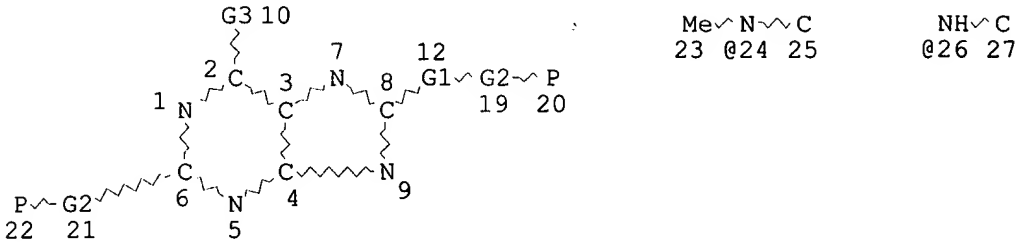
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE
L32 0 SEA FILE=REGISTRY SSS FUL L26

100.0% PROCESSED 48088 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.07

Searched by: Mary Hale 308-4258 CM-1 1E01

=> d l39 que stat;d l40 que stat;d l41 que stat
L35 STR



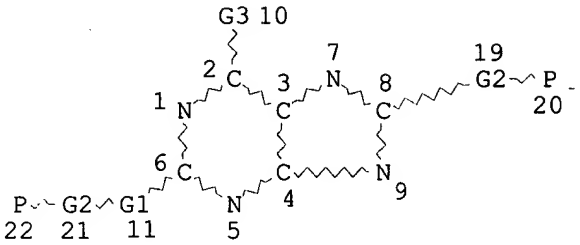
VAR G1=X/O/S/N/C
REP G2=(0-20) A
VAR G3=NH2/24/26
NODE ATTRIBUTES:
NSPEC IS RC AT 25
NSPEC IS RC AT 27
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L39 0 SEA FILE=REGISTRY SSS FUL L35

100.0% PROCESSED 28877 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.04

L34 STR



VAR G1=X/O/S/N/C
REP G2=(0-20) A
VAR G3=NH2/26/28
NODE ATTRIBUTES:
NSPEC IS RC AT 27
NSPEC IS RC AT 29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

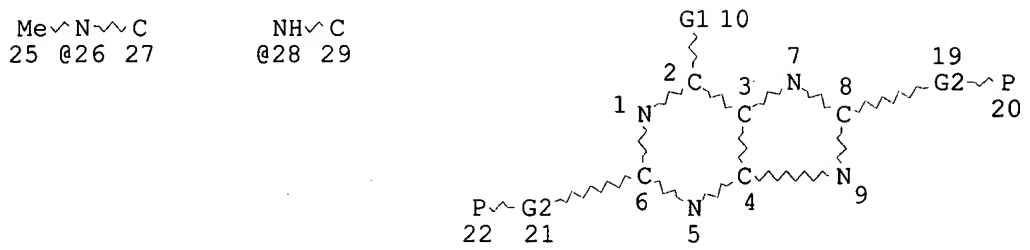
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 20

STEREO ATTRIBUTES: NONE
L40 0 SEA FILE=REGISTRY SSS FUL L34

Searched by: Mary Hale 308-4258 CM-1 1E01

100.0% PROCESSED 28877 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

L33 STR



VAR G1=NH2/26/28
REP G2=(0-20) A
NODE ATTRIBUTES:
NSPEC IS RC AT 27
NSPEC IS RC AT 29
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 19

STEREO ATTRIBUTES: NONE
L41 0 SEA FILE=REGISTRY SSS FUL L33

100.0% PROCESSED 51227 ITERATIONS 0 ANSWERS
SEARCH TIME: 00.00.03

=> fil caol;dis his

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2113.84	2114.05

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-33.04	-33.04

FILE 'CAOLD' ENTERED AT 13:42:39 ON 20 JUN 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907-1966
FILE LAST UPDATED: 01 May 1997 (19970501/UP)

This file contains CAS Registry Numbers for easy and accurate substance identification. Title keywords, authors, patent assignees, and patent information, e.g., patent numbers, are now searchable from 1907-1966. TIFF images of CA abstracts printed between 1907-1966 are available in the PAGE display formats.

Searched by: Mary Hale 308-4258 CM-1 1E01

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

(FILE 'HOME' ENTERED AT 13:27:43 ON 20 JUN 2002)

FILE 'REGISTRY' ENTERED AT 13:27:49 ON 20 JUN 2002

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L1               STR
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L2               STR L1
L3             0 S L2
L4             0 S L2 FUL
L5               STR L2
L6             0 S L5
L7             0 S L5 FUL
L8               STR L2
L9             0 S L8
L10            0 S L8 FUL
L11              STR L8
L12            0 S L11
L13            0 S L11 FUL
L14              STR L8
L15            0 S L14
L16            0 S L14 FUL
L17              STR L8
L18            0 S L17
L19            0 S L17 FUL
L20              STR L17
L21              STR L17
L22            0 S L20 OR L21
L23           57 S L20 OR L21 FUL
L24              STR L8
L25              STR L8
L26              STR L8
L27            0 S L26
L28            0 S L25
L29            0 S L24
L30            0 S L24 FUL
L31            0 S L25 FUL
L32            0 S L26 FUL
L33              STR L26
L34              STR L25
L35              STR L24
L36            0 S L35
L37            0 S L34
L38            0 S L33
L39            0 S L35 FULL
L40            0 S L34 FULL
L41            0 S L33 FULL
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FILE 'CAOLD' ENTERED AT 13:42:39 ON 20 JUN 2002

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=> s l23
L42           0 L23

=> fil hca;s l23
COST IN U.S. DOLLARS                        SINCE FILE      TOTAL
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Searched by: Mary Hale 308-4258 CM-1 1E01

	ENTRY	SESSION
FULL ESTIMATED COST	0.38	2114.43

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-33.04

FILE 'HCA' ENTERED AT 13:42:47 ON 20 JUN 2002
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1907 - 13 Jun 2002 VOL 136 ISS 25
FILE LAST UPDATED: 13 Jun 2002 (20020613/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

L43 16 L23

=> log y

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	2.04	2116.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-33.04

STN INTERNATIONAL LOGOFF AT 13:42:51 ON 20 JUN 2002

Searched by: Mary Hale 308-4258 CM-1 1E01